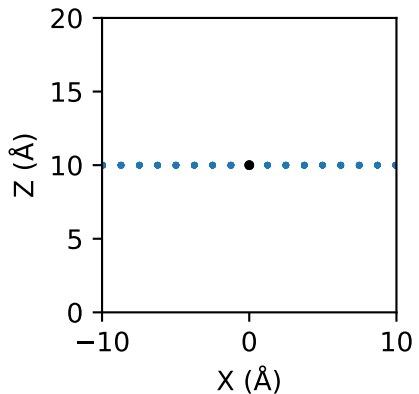
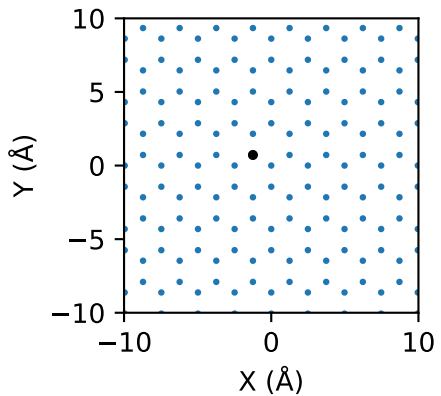


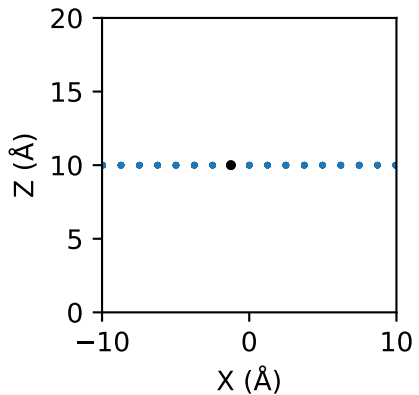
Distance = 0.0 Å  
Cell vector (Rx, Ry, Rz) = (0, 0, 0)  
Cartesian vector (rx, ry, rz) = (0.0, 0.0, 0.0)  
Atomic index (A1, A2) = (1, 1)  
from atom 1 to atom 1  
Hamiltonian Unit: meV



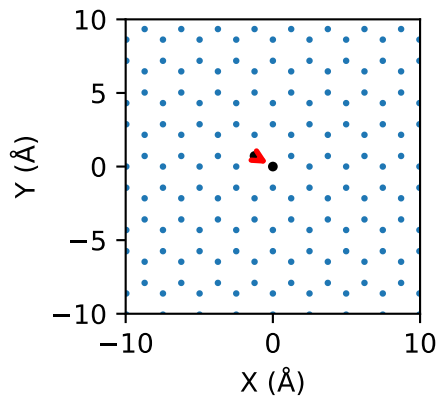
	pz
pz	-2517.908



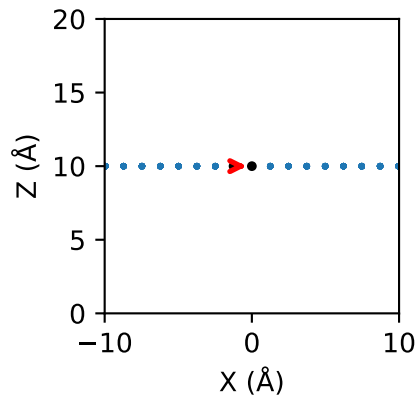
Distance = 0.0 Å  
Cell vector (Rx, Ry, Rz) = (0, 0, 0)  
Cartesian vector (rx, ry, rz) = (0.0, 0.0, 0.0)  
Atomic index (A1, A2) = (2, 2)  
from atom 2 to atom 2  
Hamiltonian Unit: meV



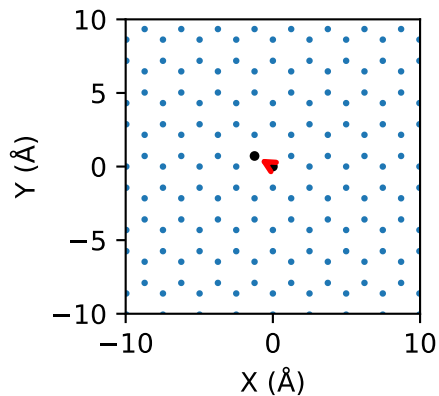
	pz
pz	-2517.908



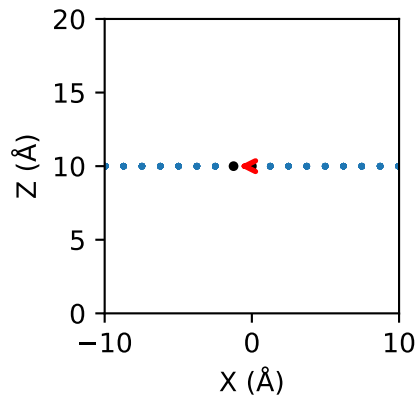
Distance = 1.437 Å  
 Cell vector (Rx, Ry, Rz) = (0, 0, 0)  
 Cartesian vector (rx, ry, rz) = (1.244, -0.718, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



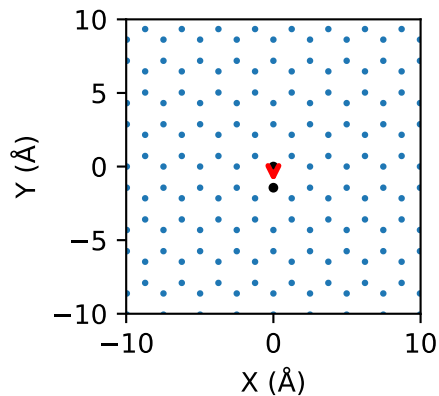
	pz
pz	-2830.899



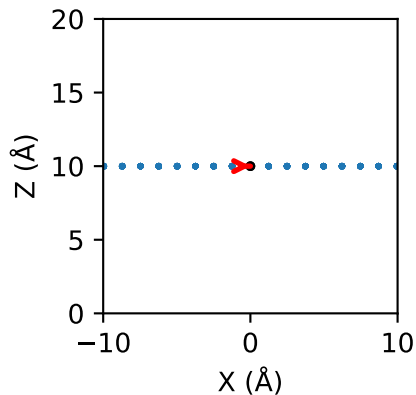
Distance = 1.437 Å  
 Cell vector (Rx, Ry, Rz) = (0, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-1.244, 0.718, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



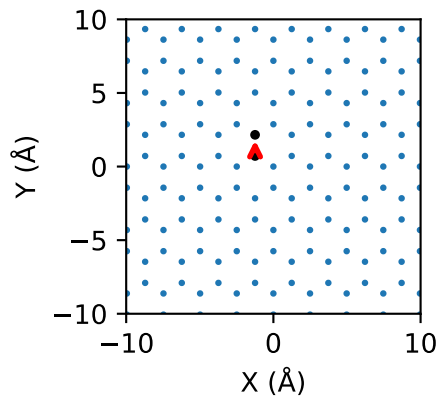
	pz
pz	-2830.899



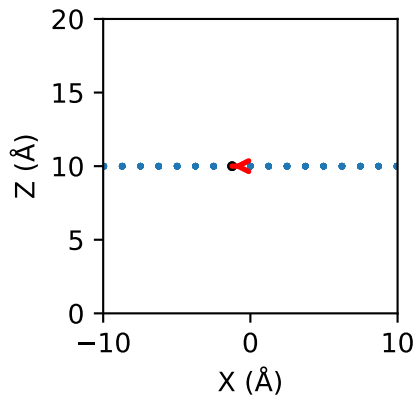
Distance = 1.437 Å  
 Cell vector (Rx, Ry, Rz) = (0, -1, 0)  
 Cartesian vector (rx, ry, rz) = (0.0, -1.437, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



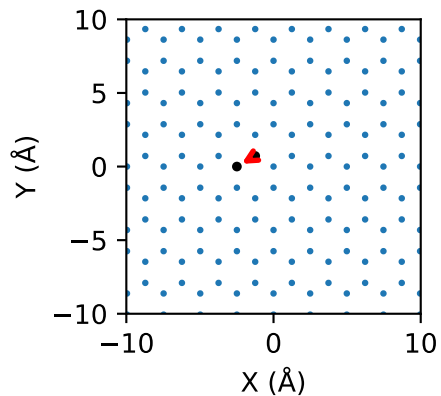
	pz
pz	11.584



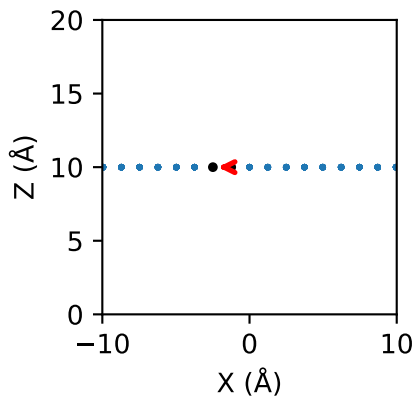
Distance = 1.437 Å  
 Cell vector (Rx, Ry, Rz) = (0, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-0.0, 1.437, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



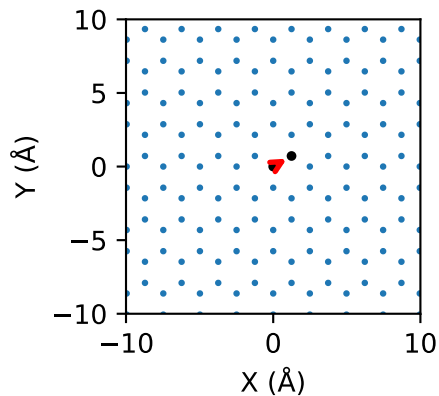
	pz
pz	11.584



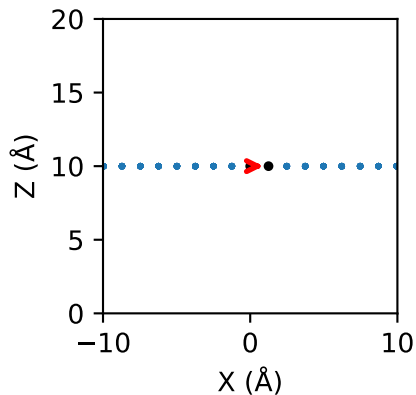
Distance = 1.437 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, -0.718, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	11.577

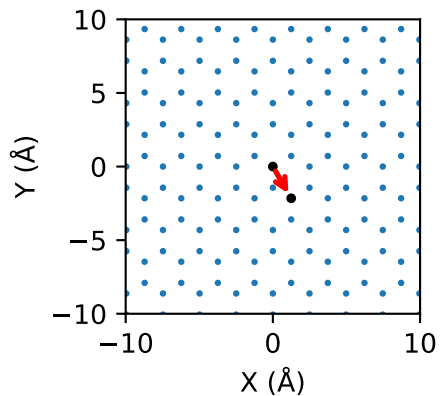


Distance = 1.437 Å  
 Cell vector (Rx, Ry, Rz) = (1, 0, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, 0.718, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

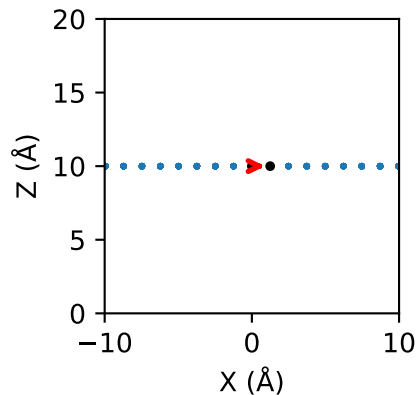


	pz
pz	11.577

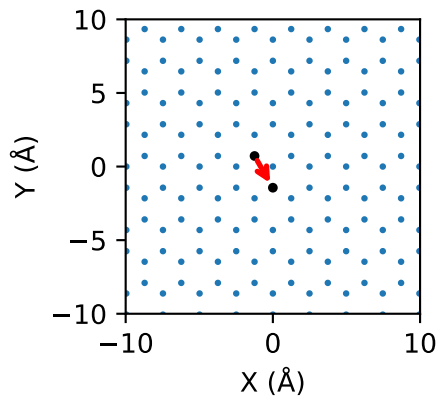




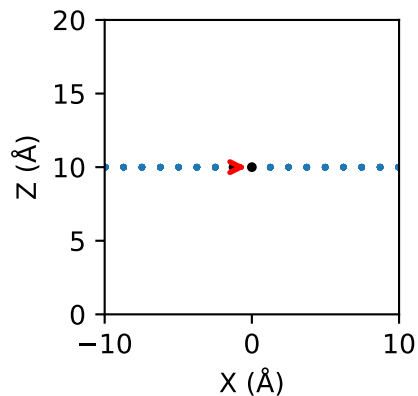
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (0, -1, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, -2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



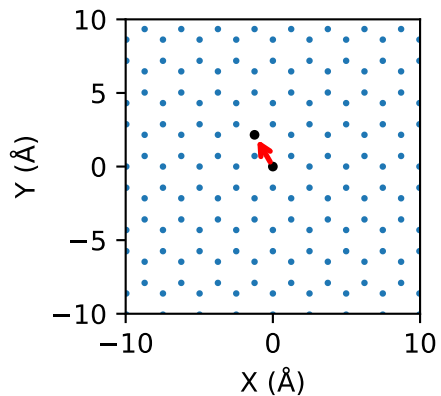
	pz
pz	238.166



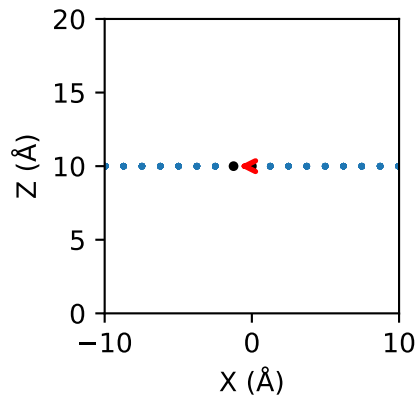
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (0, -1, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, -2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



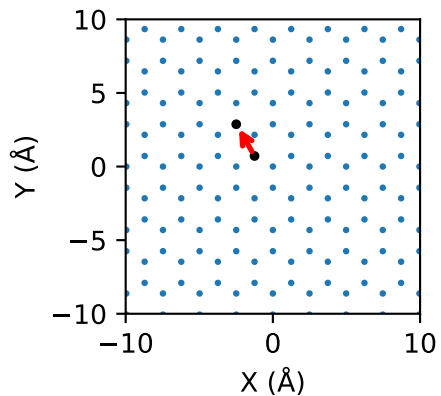
	pz
pz	238.166



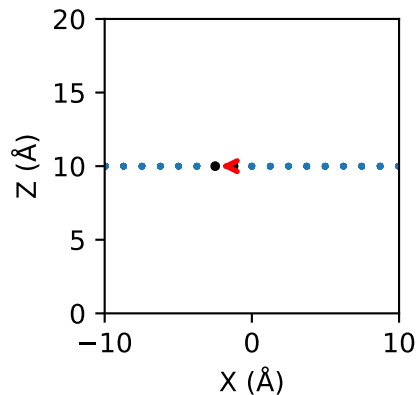
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (0, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, 2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



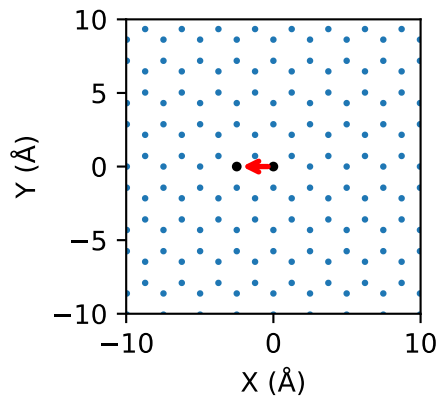
	pz
pz	238.166



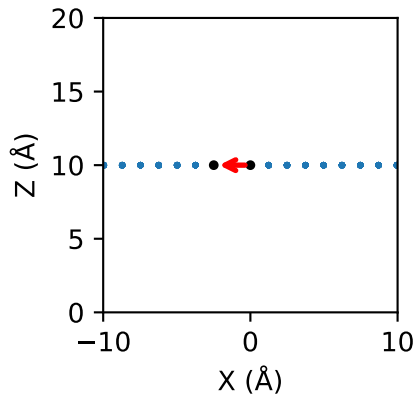
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (0, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, 2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



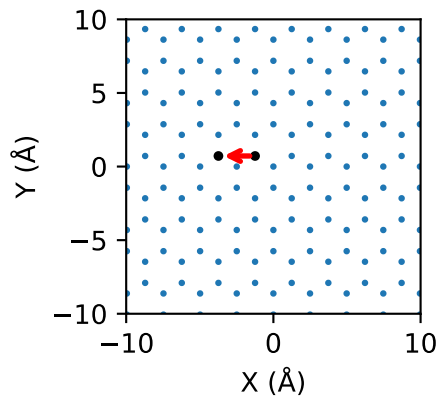
	pz
pz	238.166



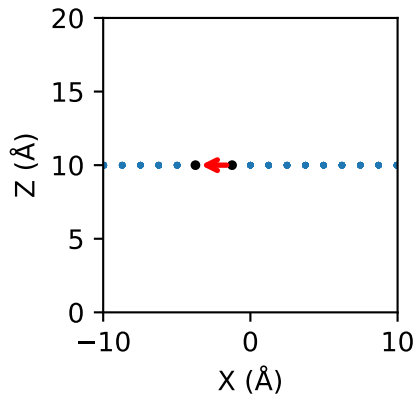
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 0.0, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



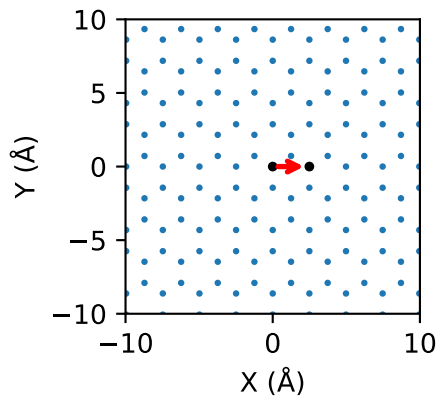
	pz
pz	238.216



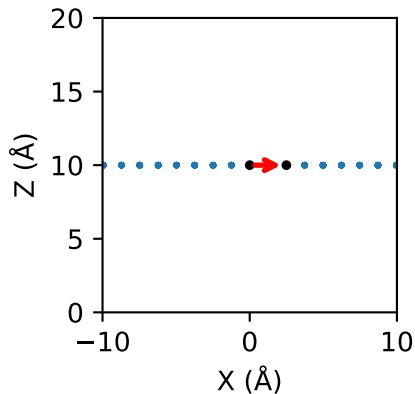
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 0.0, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



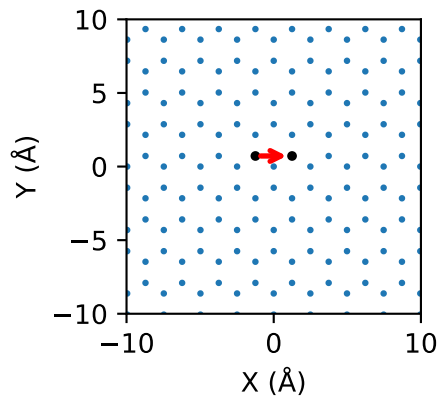
	pz
pz	238.216



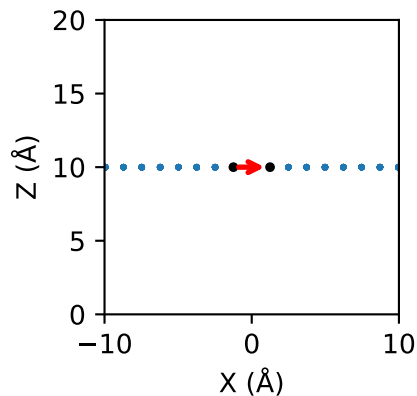
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (1, 0, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 0.0, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	238.216

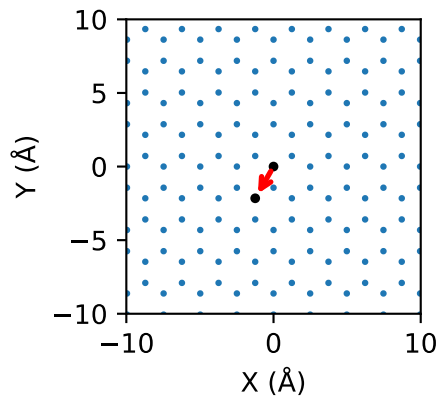


Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (1, 0, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 0.0, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

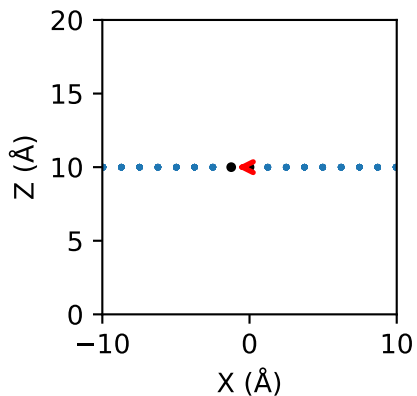


	pz
pz	238.216

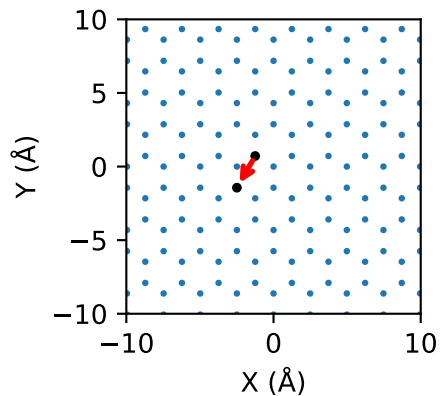




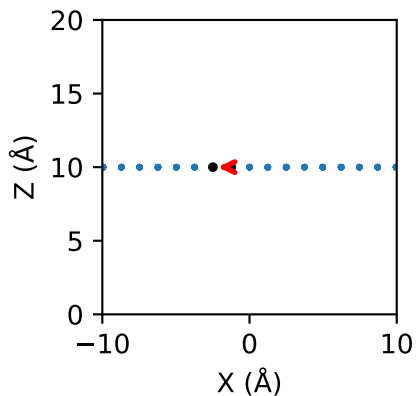
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (-1, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, -2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



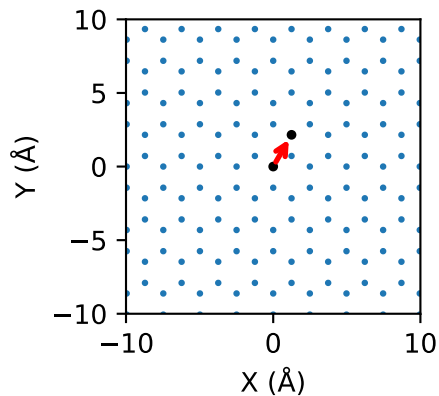
	pz
pz	238.116



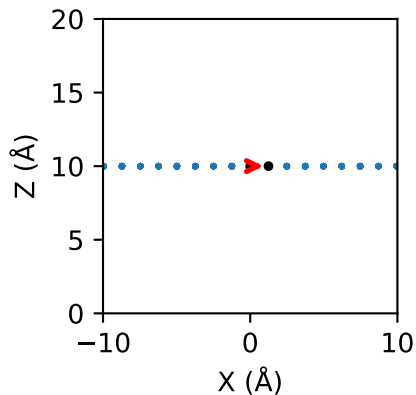
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (-1, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, -2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



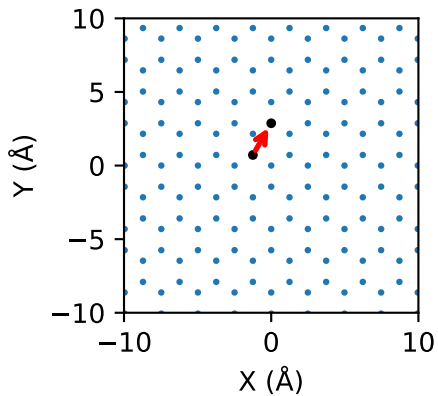
	pz
pz	238.116



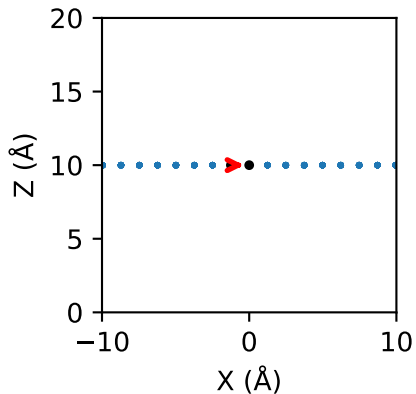
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (1, 1, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, 2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



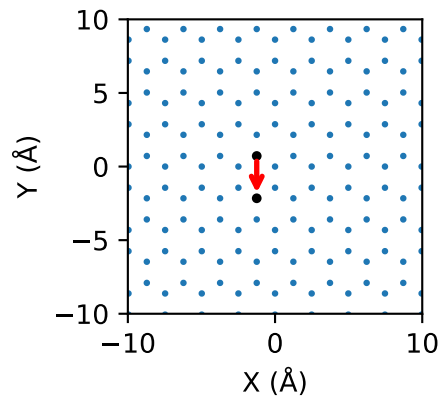
	pz
pz	238.116



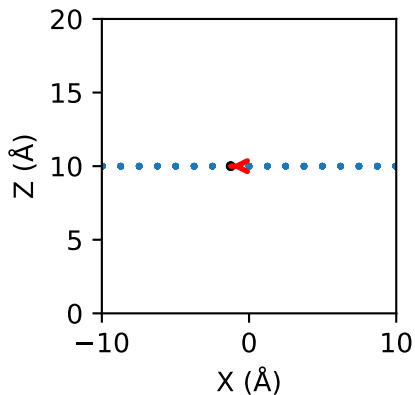
Distance = 2.489 Å  
 Cell vector (Rx, Ry, Rz) = (1, 1, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, 2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



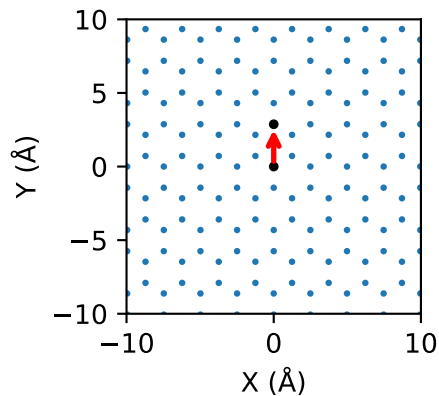
	pz
pz	238.116



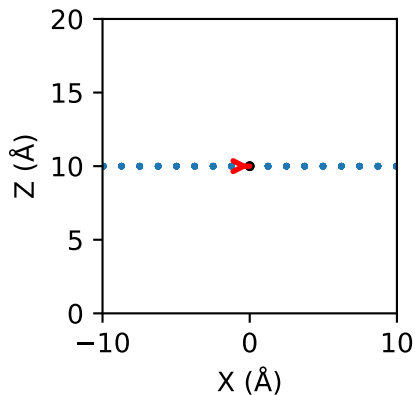
Distance =  $2.874 \text{ \AA}$   
 Cell vector ( $R_x, R_y, R_z$ ) =  $(-1, -1, 0)$   
 Cartesian vector ( $r_x, r_y, r_z$ ) =  $(-0.0, -2.874, 0.0)$   
 Atomic index ( $A_1, A_2$ ) =  $(1, 2)$   
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



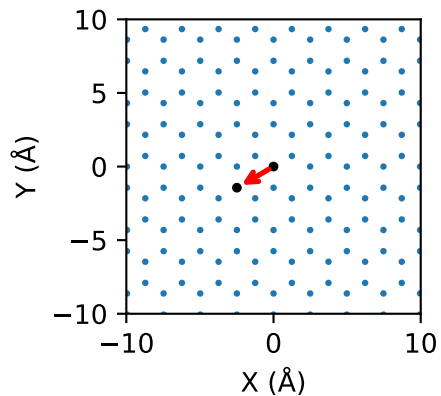
	pz
pz	-247.29



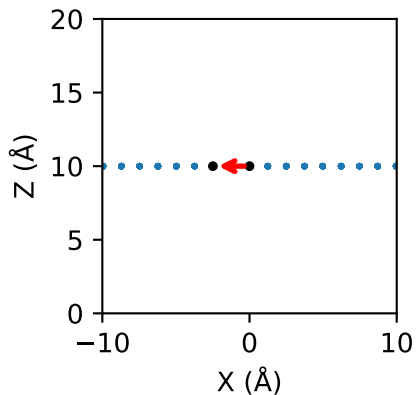
Distance = 2.874 Å  
 Cell vector (Rx, Ry, Rz) = (1, 1, 0)  
 Cartesian vector (rx, ry, rz) = (0.0, 2.874, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



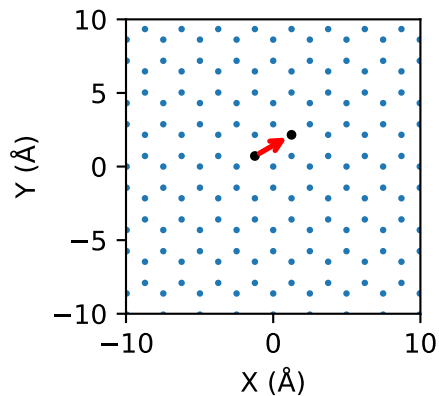
	pz
pz	-247.29



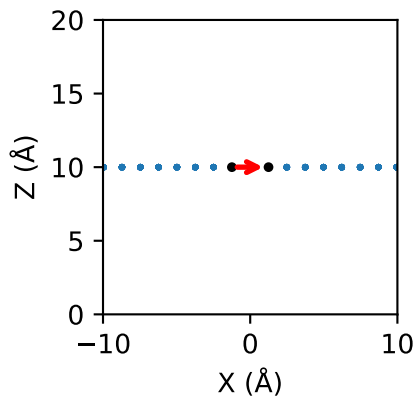
Distance = 2.874 Å  
 Cell vector (Rx, Ry, Rz) = (-1, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, -1.437, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



	pz
pz	-247.307

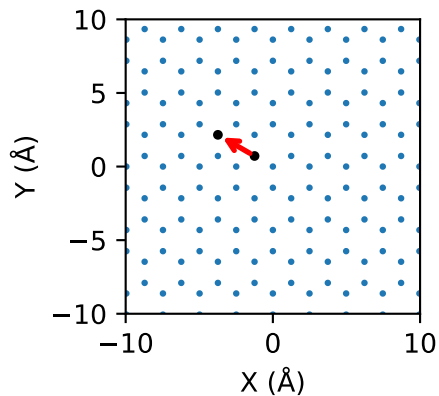


Distance = 2.874 Å  
 Cell vector (Rx, Ry, Rz) = (1, 1, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 1.437, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV

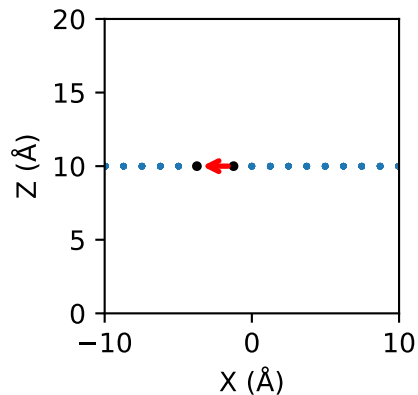


	pz
pz	-247.307

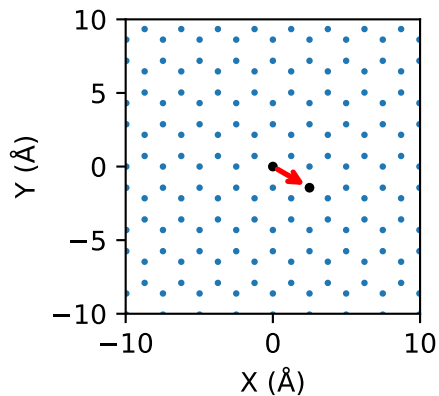




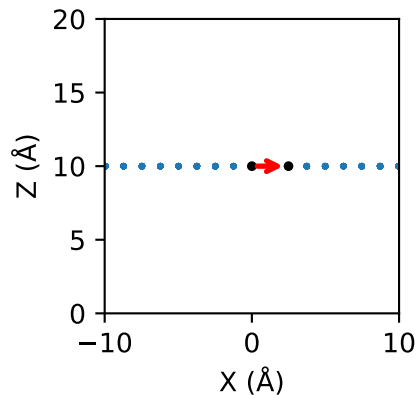
Distance = 2.874 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 1.437, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



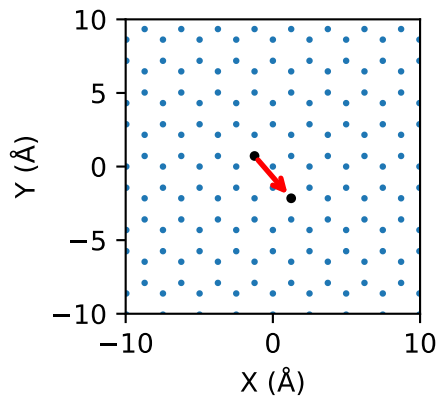
	pz
pz	-22.279



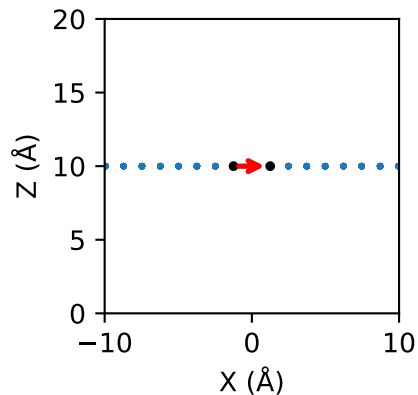
Distance = 2.874 Å  
 Cell vector (Rx, Ry, Rz) = (1, -1, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, -1.437, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



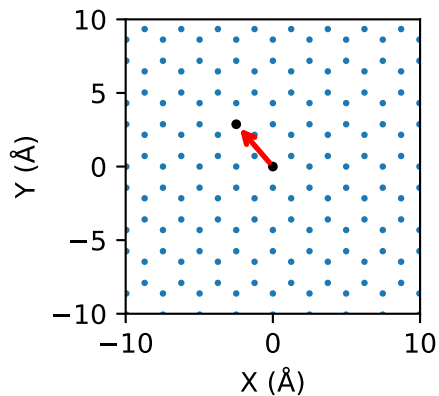
	pz
pz	-22.279



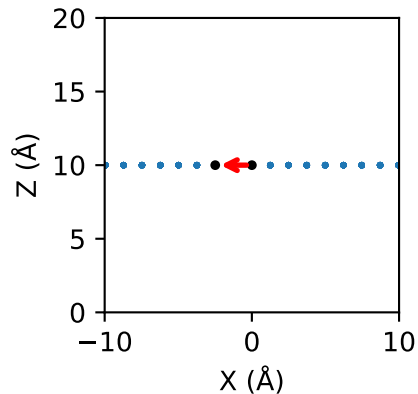
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (0, -1, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, -2.874, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



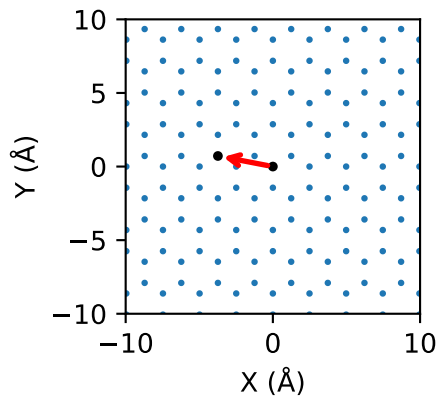
	pz
pz	-2830.21



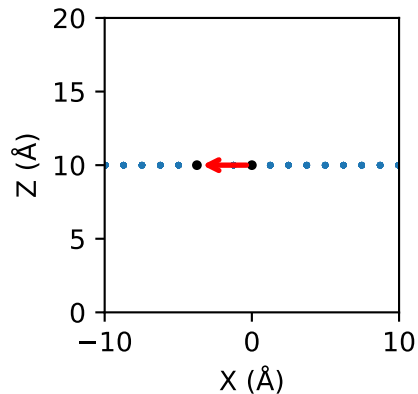
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (0, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 2.874, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



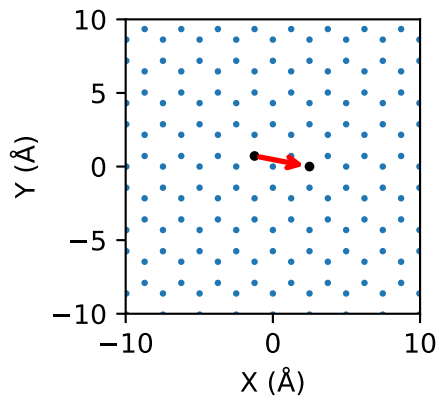
	pz
pz	-2830.21



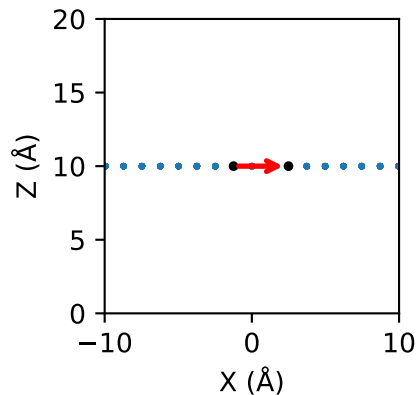
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-3.733, 0.718, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



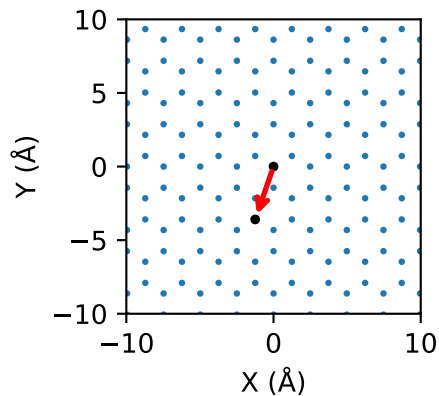
	pz
pz	-2830.551



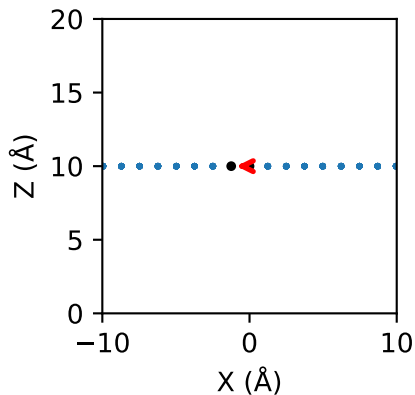
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (1, 0, 0)  
 Cartesian vector (rx, ry, rz) = (3.733, -0.718, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



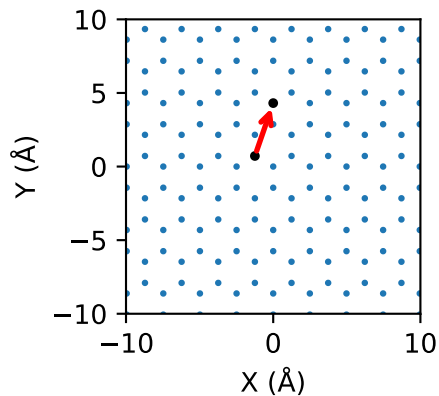
	pz
pz	-2830.551



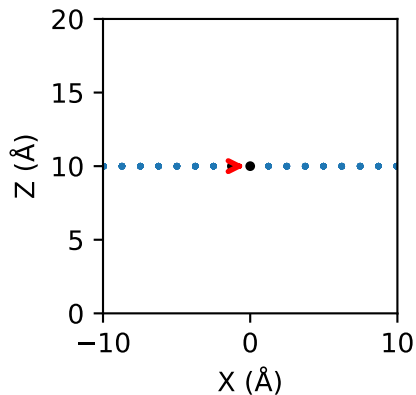
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (-1, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-1.244, -3.593, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



	pz
pz	-9.703

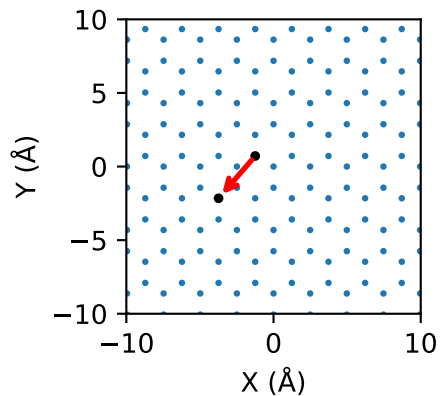


Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (1, 2, 0)  
 Cartesian vector (rx, ry, rz) = (1.244, 3.593, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV

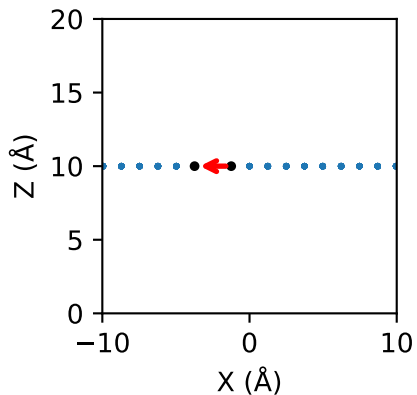


	pz
pz	-9.703

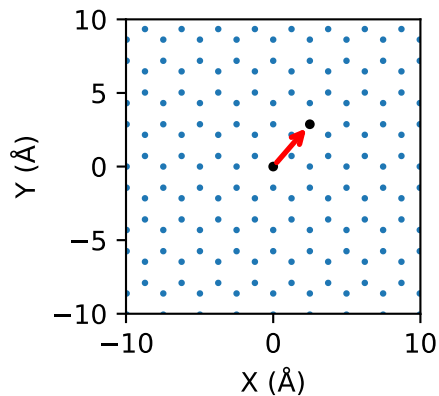




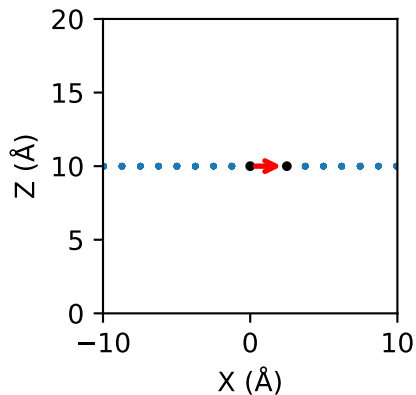
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, -2.874, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



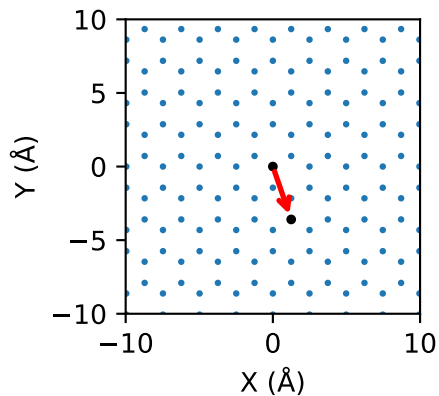
	pz
pz	-9.707



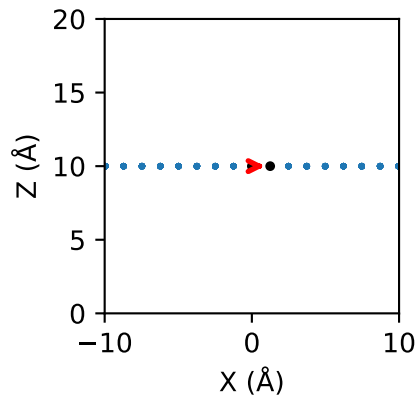
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (2, 1, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 2.874, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



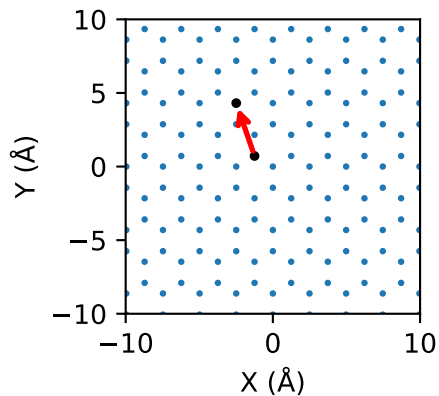
	pz
pz	-9.707



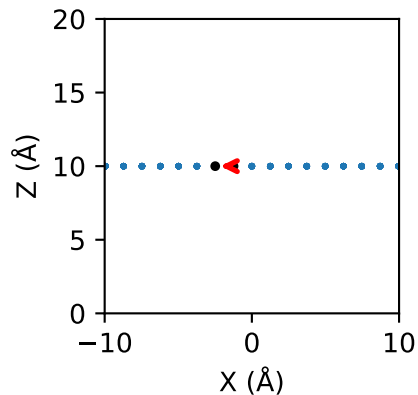
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (0, -2, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, -3.593, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



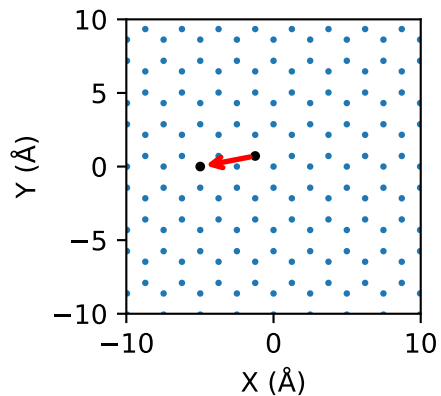
	pz
pz	6.172



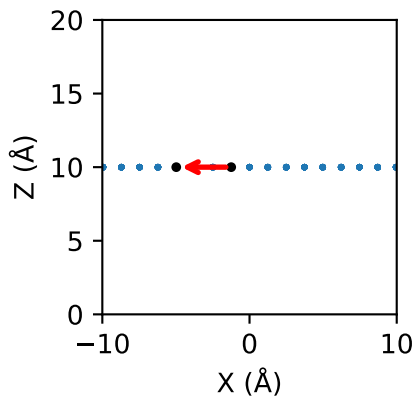
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (0, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, 3.593, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



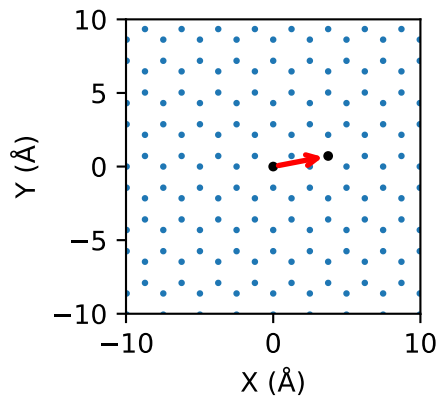
	pz
pz	6.172



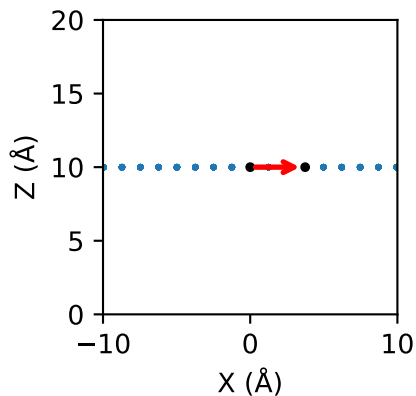
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, -0.718, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



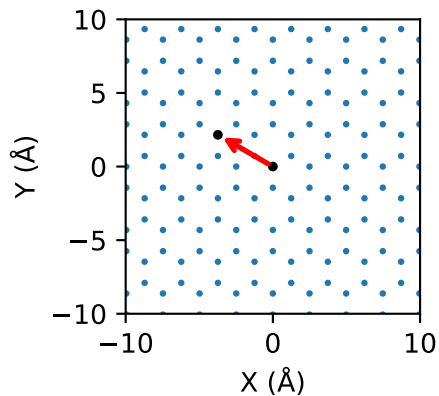
	pz
pz	6.173



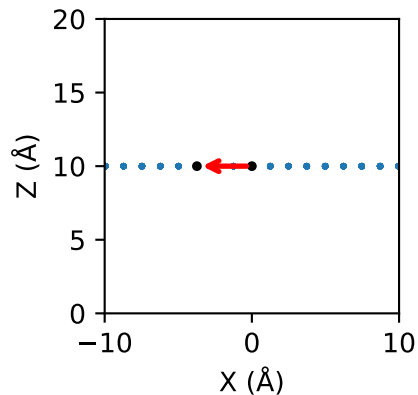
Distance = 3.802 Å  
 Cell vector (Rx, Ry, Rz) = (2, 0, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, 0.718, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



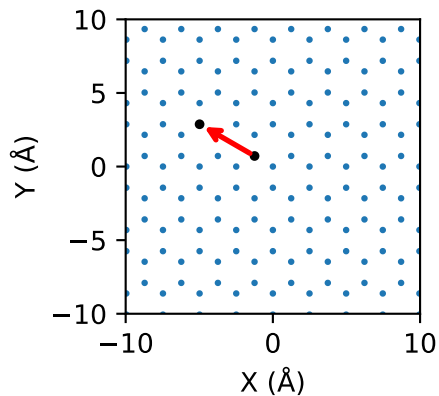
	pz
pz	6.173



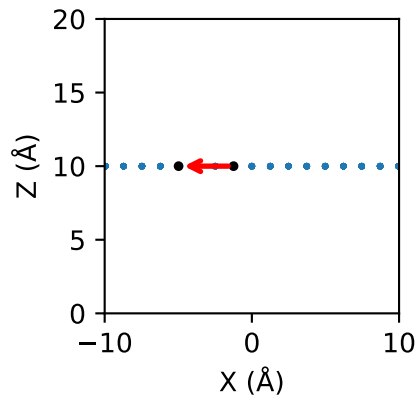
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, 2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	50.812

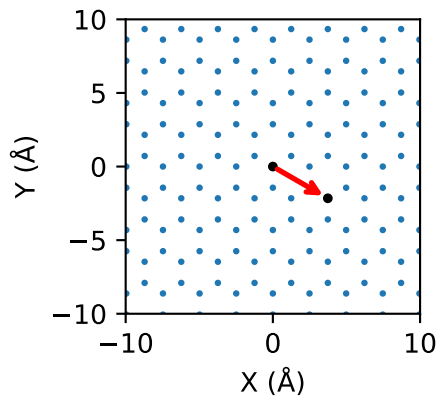


Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, 2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

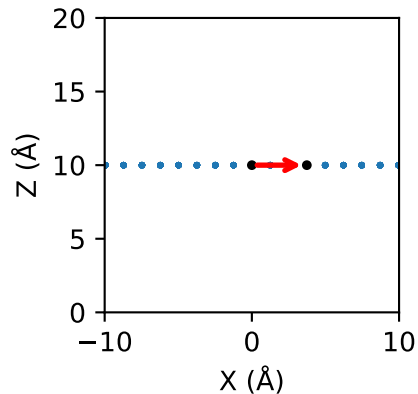


	pz
pz	50.812

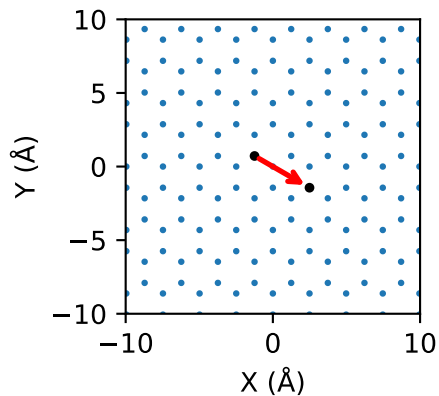




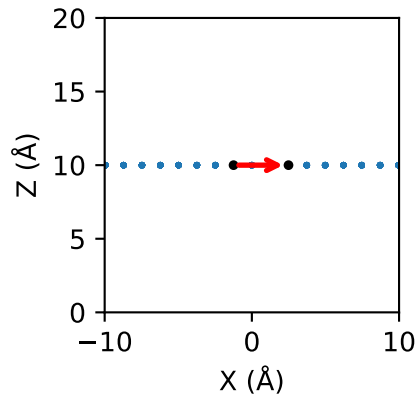
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (1, -1, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, -2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



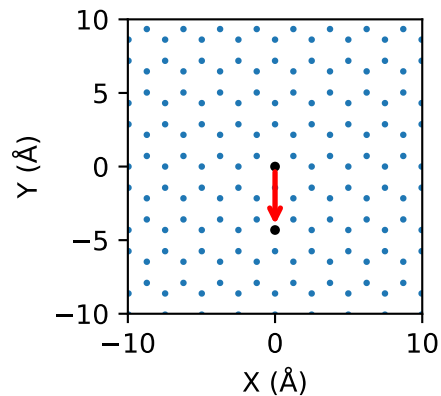
	pz
pz	50.812



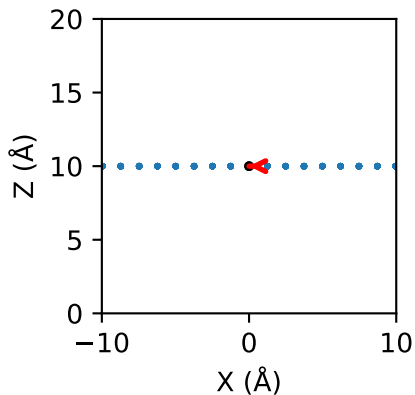
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (1, -1, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, -2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



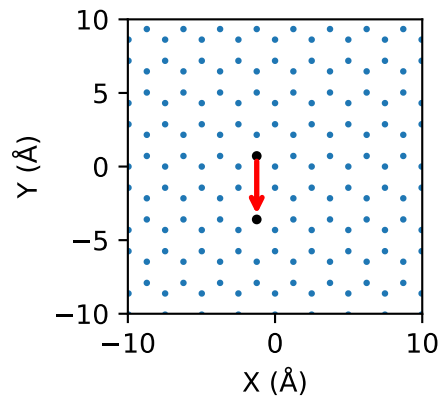
	pz
pz	50.812



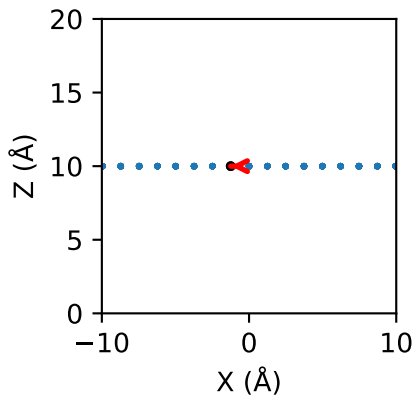
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (-1, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-0.0, -4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



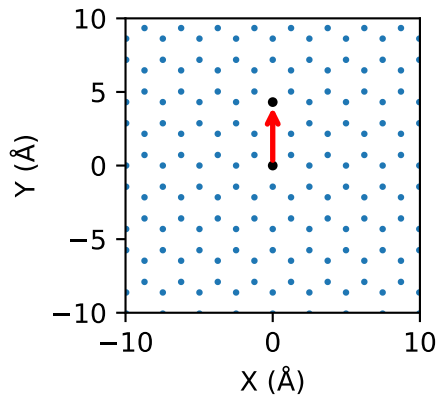
	pz
pz	50.797



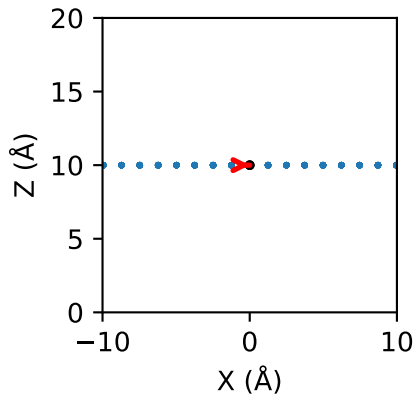
Distance = 4.311 Å  
 Cell vector ( $R_x, R_y, R_z$ ) = (-1, -2, 0)  
 Cartesian vector ( $r_x, r_y, r_z$ ) = (-0.0, -4.311, 0.0)  
 Atomic index ( $A_1, A_2$ ) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



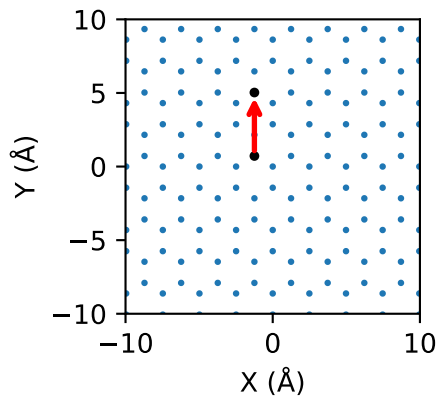
	pz
pz	50.797



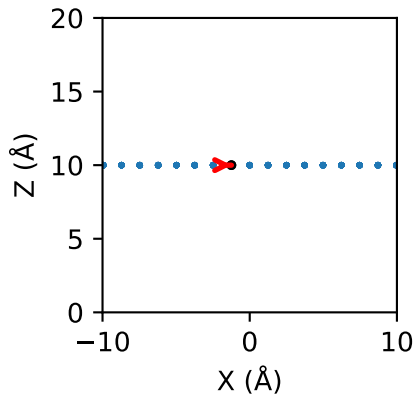
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (1, 2, 0)  
 Cartesian vector (rx, ry, rz) = (0.0, 4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



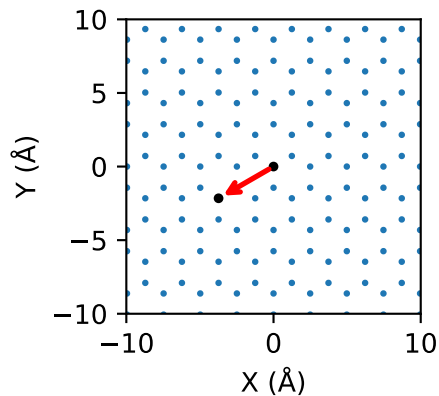
	pz
pz	50.797



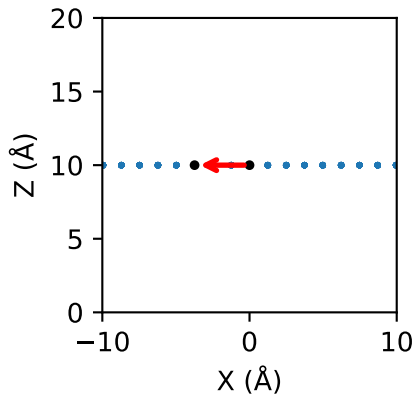
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (1, 2, 0)  
 Cartesian vector (rx, ry, rz) = (0.0, 4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



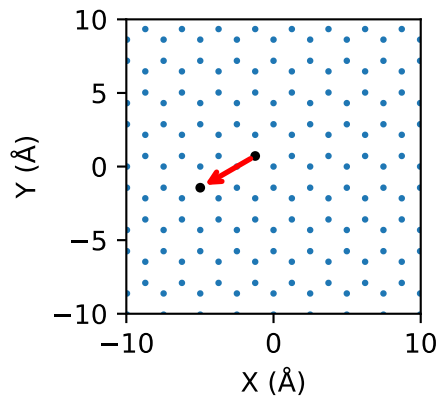
	pz
pz	50.797



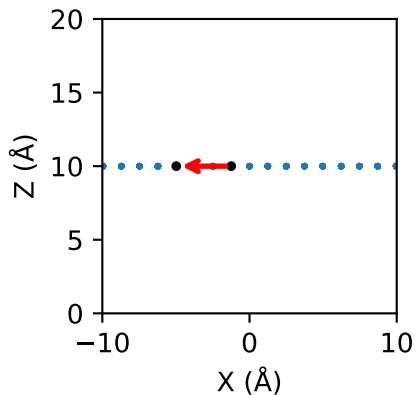
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, -2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	50.804

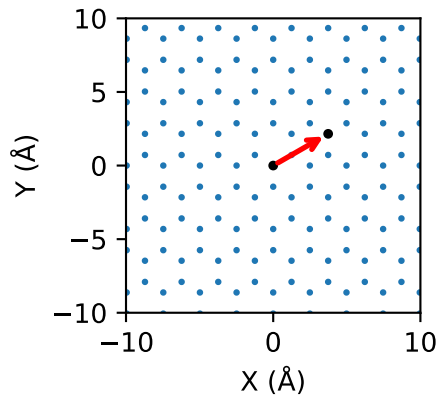


Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, -2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

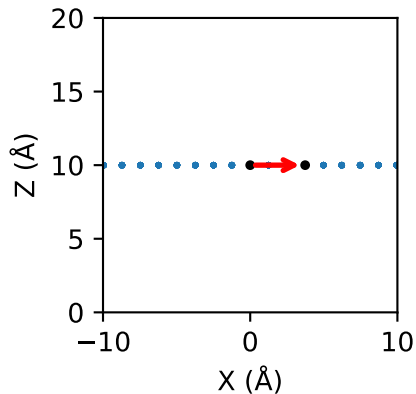


	pz
pz	50.804

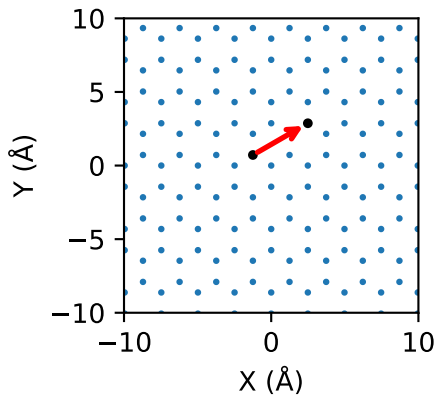




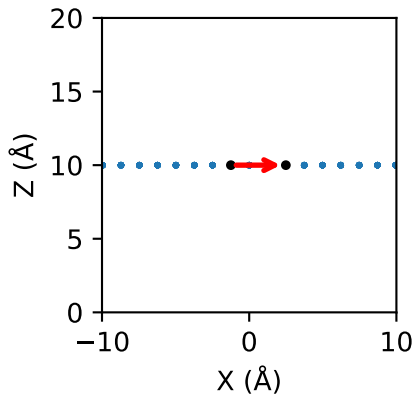
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (2, 1, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, 2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



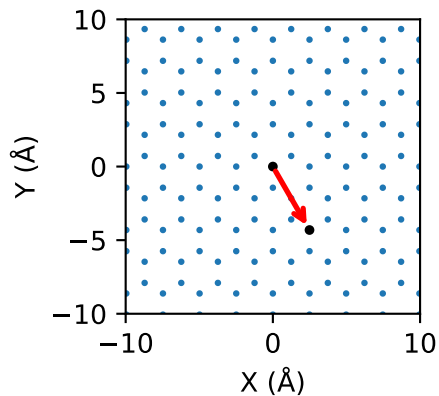
	pz
pz	50.804



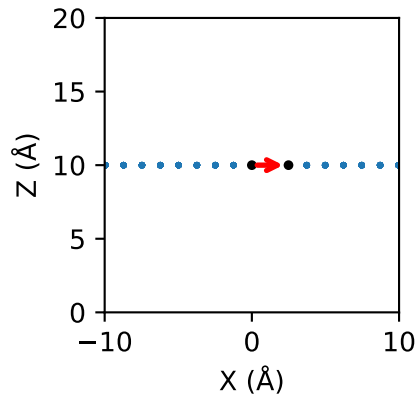
Distance = 4.311 Å  
 Cell vector (Rx, Ry, Rz) = (2, 1, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, 2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



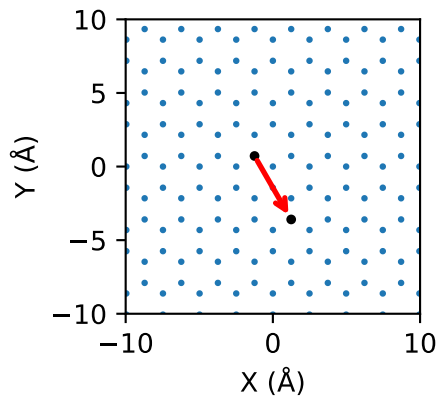
	pz
pz	50.804



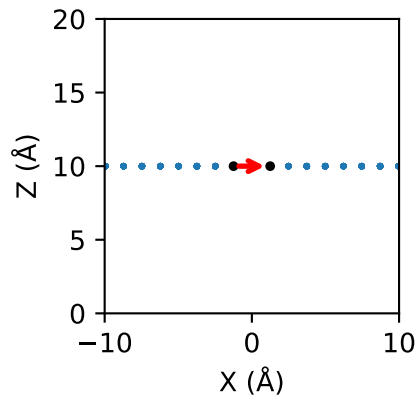
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (0, -2, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, -4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



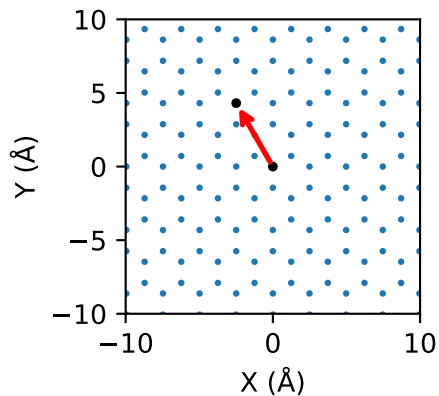
	pz
pz	-19.065



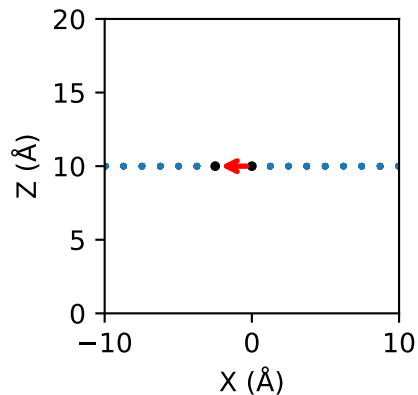
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (0, -2, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, -4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



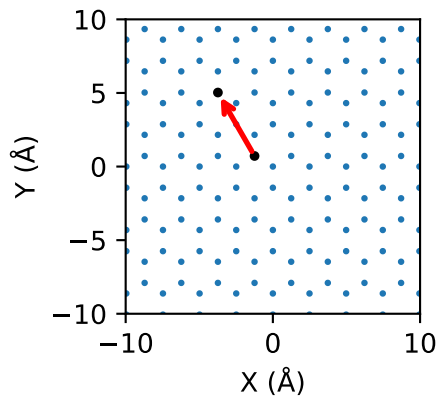
	pz
pz	-19.065



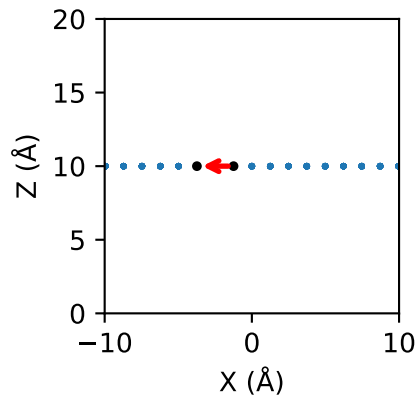
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (0, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



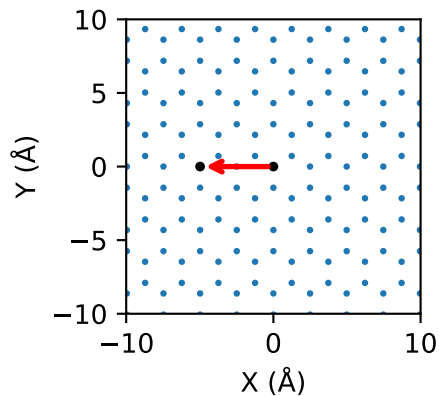
	pz
pz	-19.065



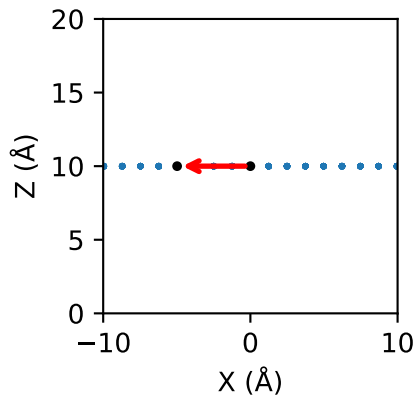
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (0, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



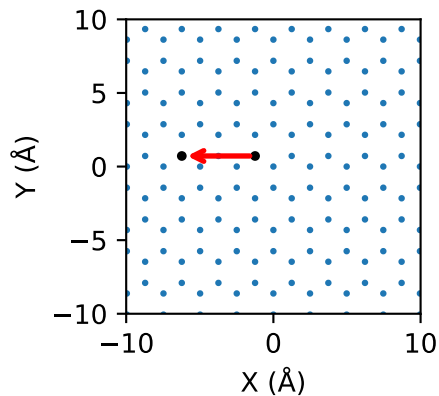
	pz
pz	-19.065



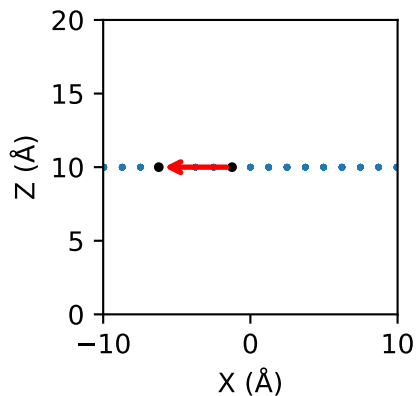
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 0.0, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-19.063

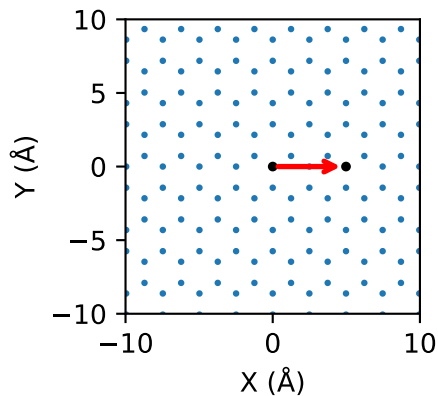


Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 0.0, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

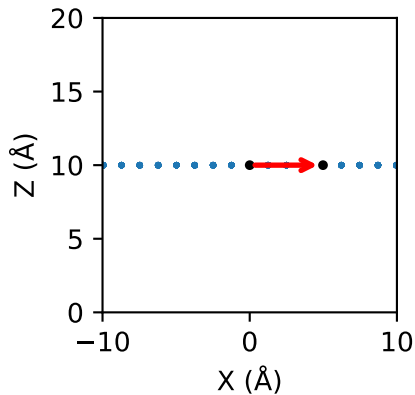


	pz
pz	-19.063

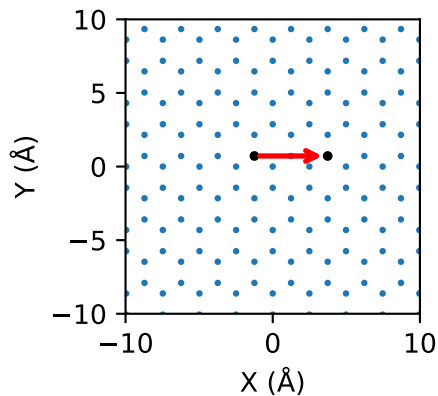




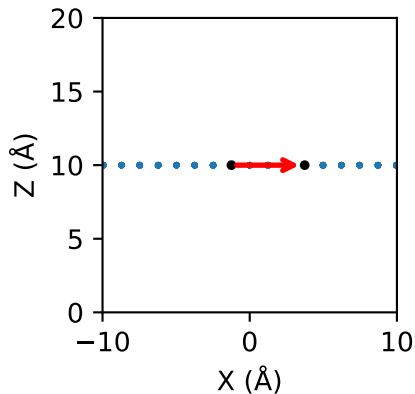
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (2, 0, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 0.0, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



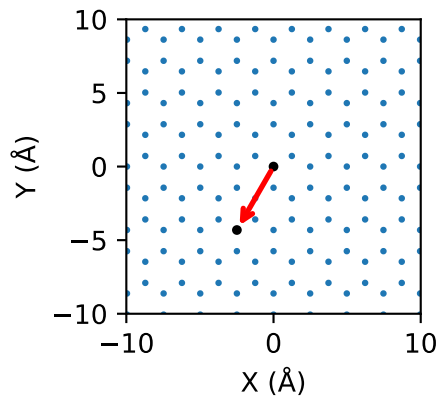
	pz
pz	-19.063



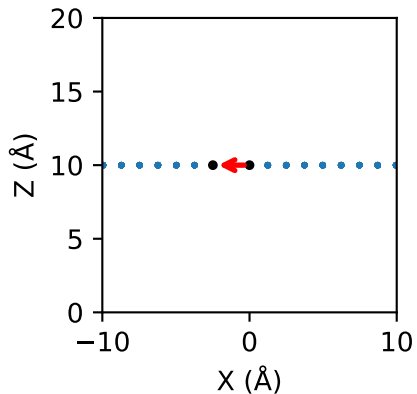
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (2, 0, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 0.0, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



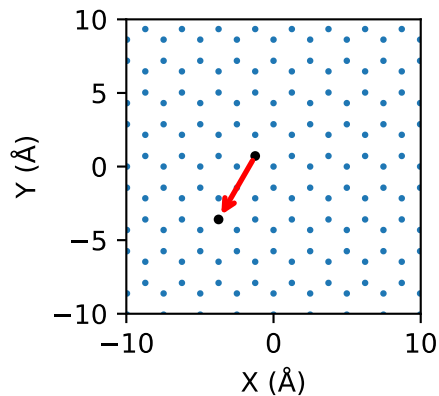
	pz
pz	-19.063



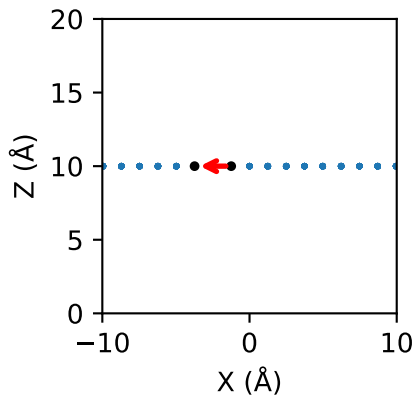
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, -4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



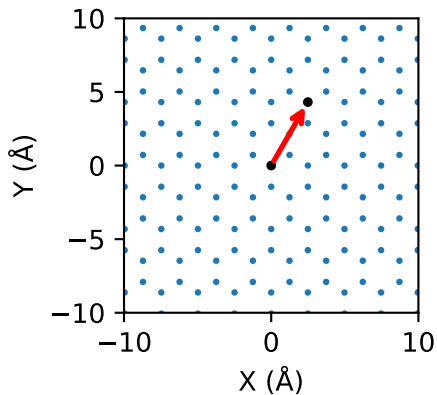
	pz
pz	-19.066



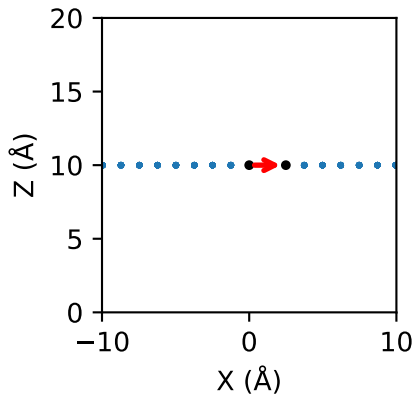
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, -4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



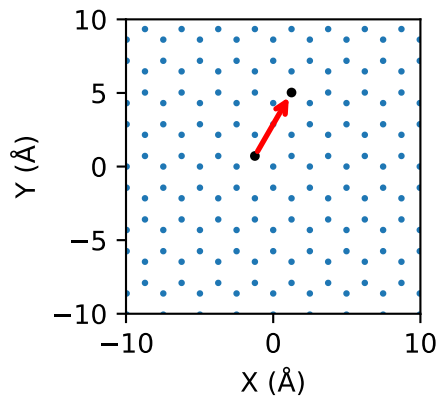
	pz
pz	-19.066



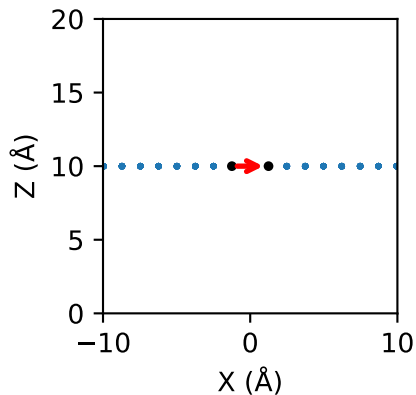
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (2, 2, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



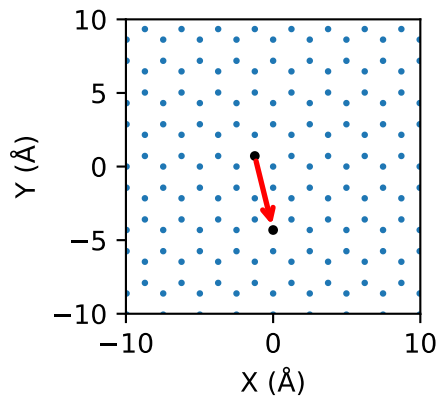
	pz
pz	-19.066



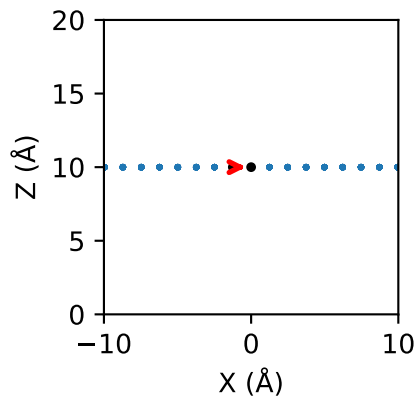
Distance = 4.978 Å  
 Cell vector (Rx, Ry, Rz) = (2, 2, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



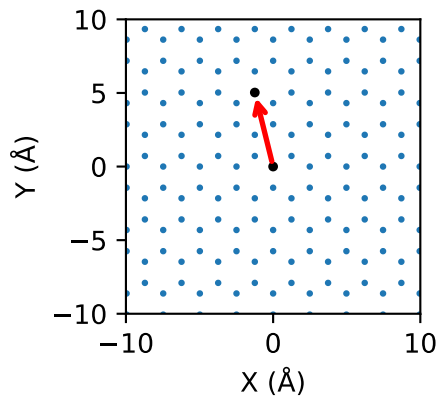
	pz
pz	-19.066



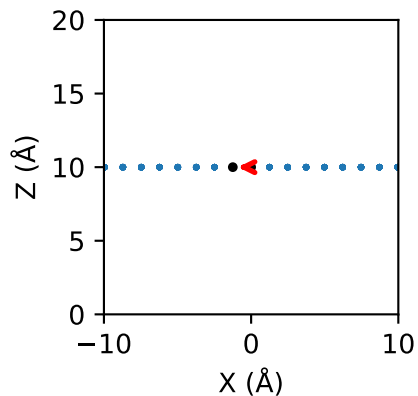
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (-1, -2, 0)  
 Cartesian vector (rx, ry, rz) = (1.244, -5.03, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	11.613

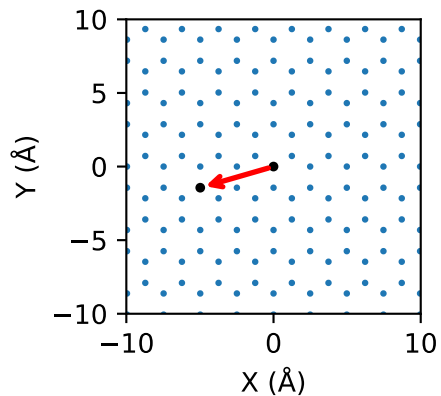


Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (1, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-1.244, 5.03, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

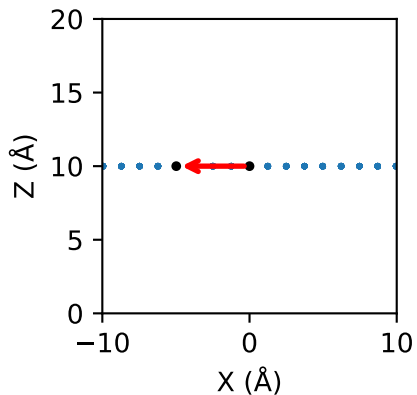


	pz
pz	11.613

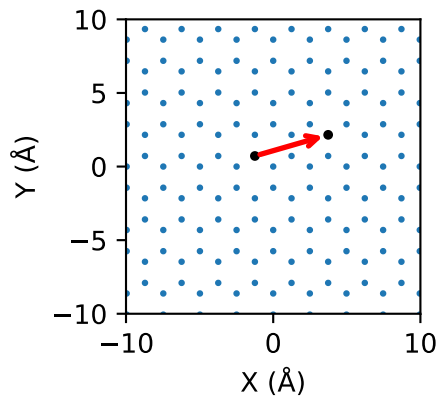




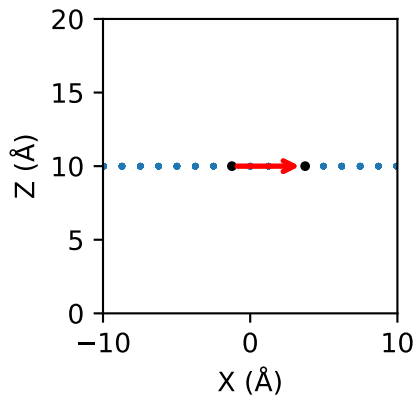
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, -1.437, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



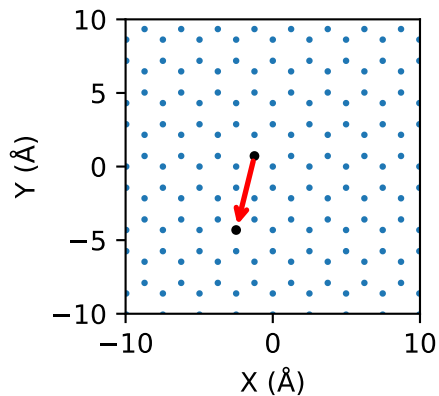
	pz
pz	11.603



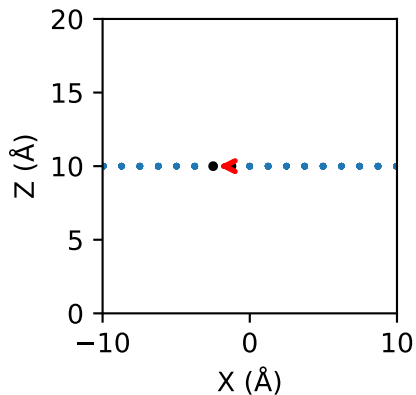
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (2, 1, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 1.437, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



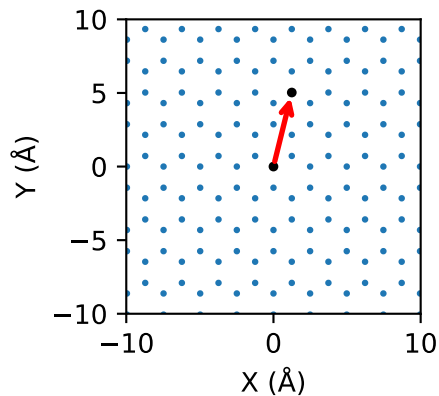
	pz
pz	11.603



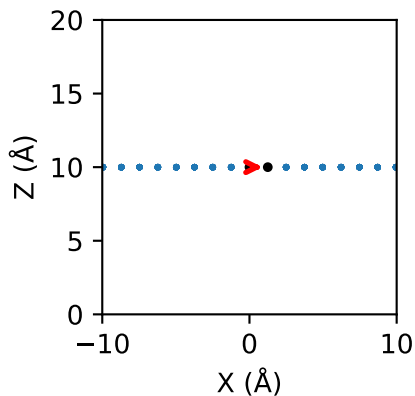
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, -5.03, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



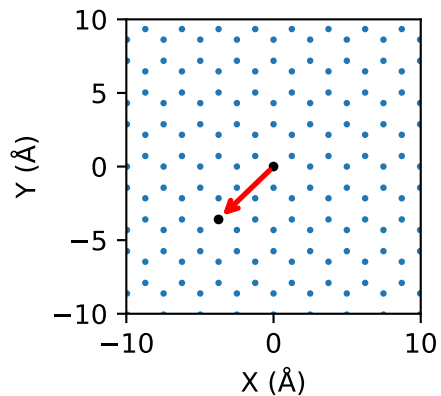
	pz
pz	-9.694



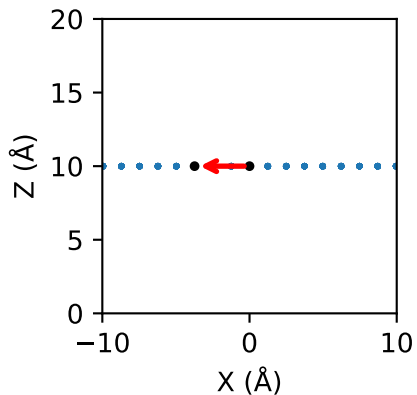
Distance =  $5.181 \text{ Å}$   
 Cell vector ( $R_x, R_y, R_z$ ) = (2, 2, 0)  
 Cartesian vector ( $r_x, r_y, r_z$ ) = (1.245, 5.03, 0.0)  
 Atomic index ( $A_1, A_2$ ) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



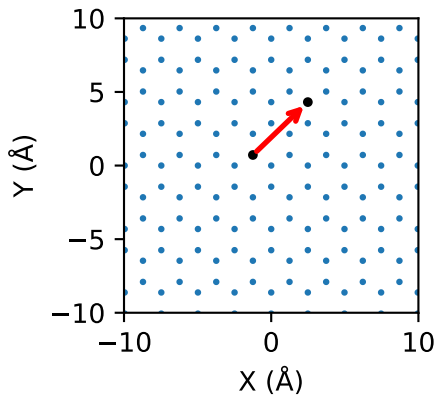
	pz
pz	-9.694



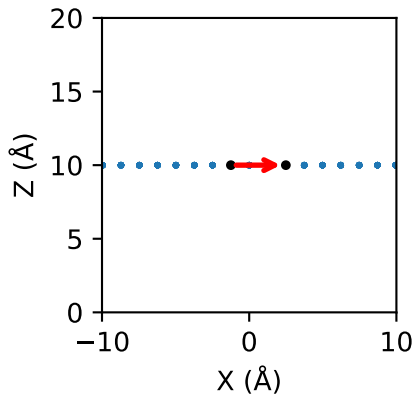
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-3.733, -3.593, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



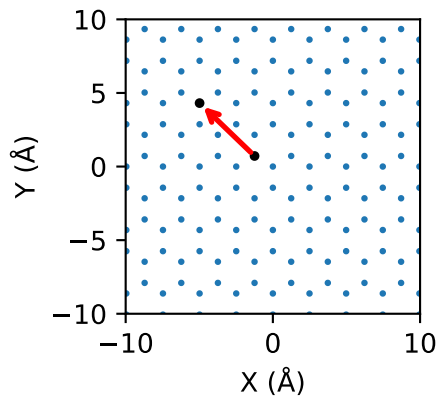
	pz
pz	-9.696



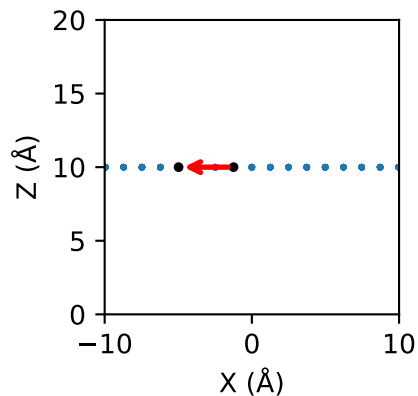
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (2, 2, 0)  
 Cartesian vector (rx, ry, rz) = (3.733, 3.593, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



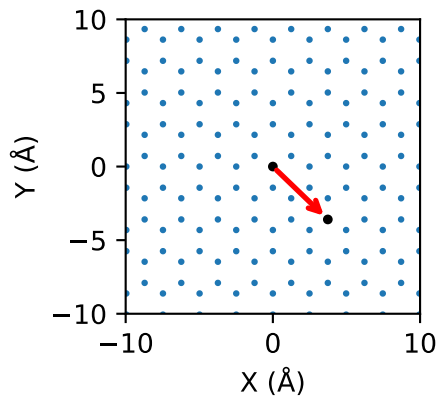
	pz
pz	-9.696



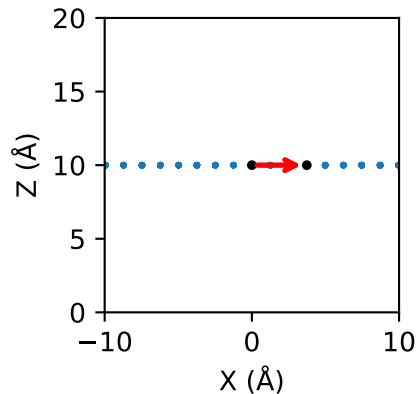
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, 3.593, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-1.48

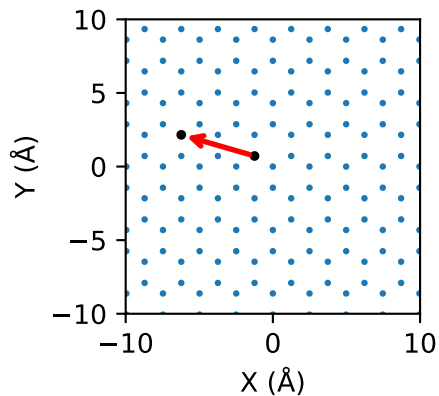


Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (1, -2, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, -3.593, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

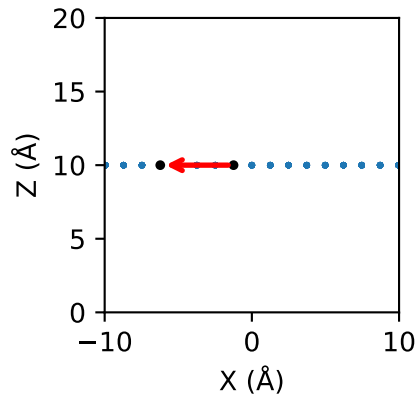


	pz
pz	-1.48

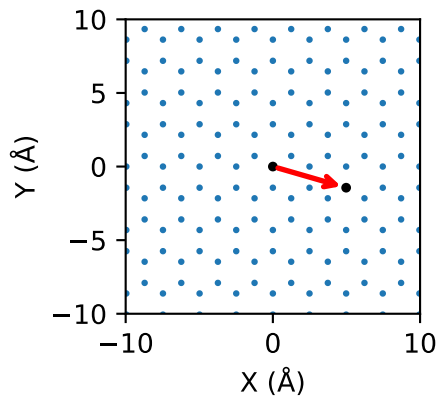




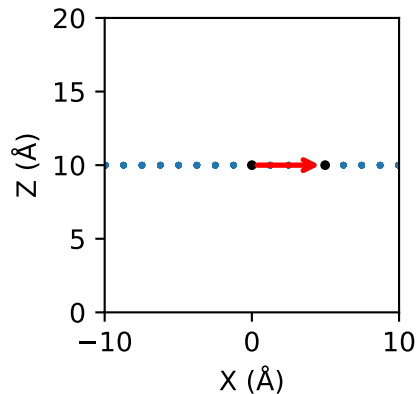
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 1.437, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



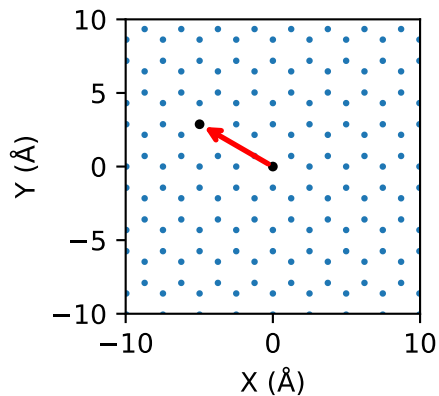
	pz
pz	-1.481



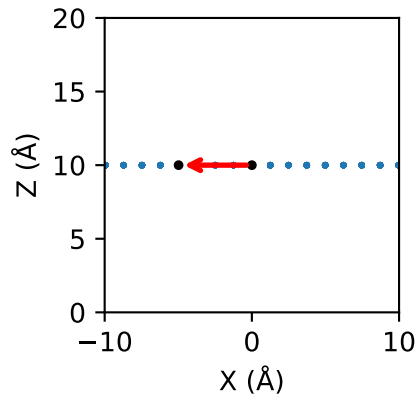
Distance = 5.181 Å  
 Cell vector (Rx, Ry, Rz) = (2, -1, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, -1.437, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



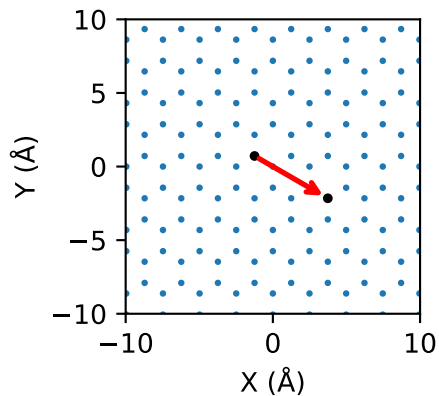
	pz
pz	-1.481



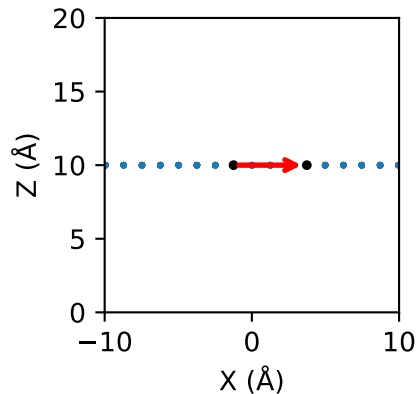
Distance = 5.748 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 2.874, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



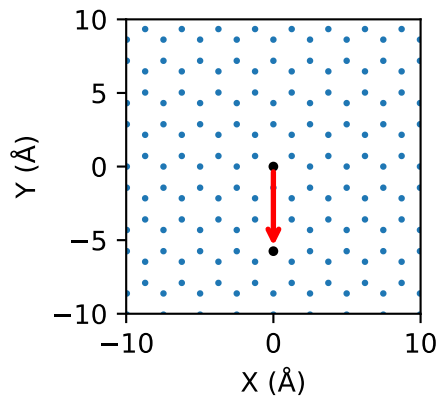
	pz
pz	-247.273



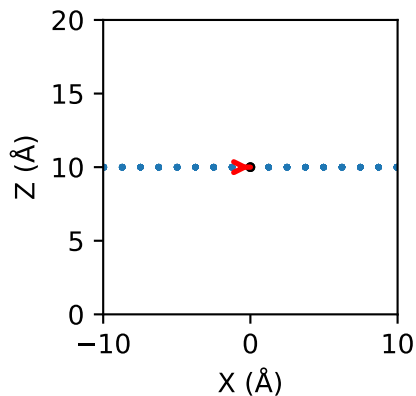
Distance = 5.748 Å  
 Cell vector (Rx, Ry, Rz) = (1, -1, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, -2.874, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



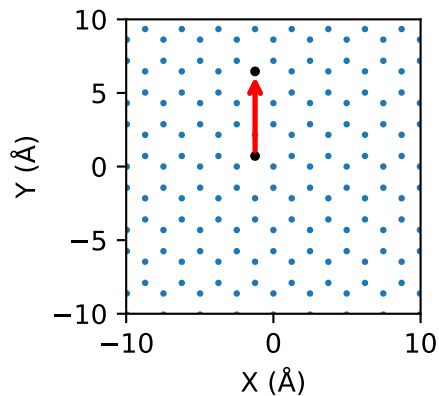
	pz
pz	-247.273



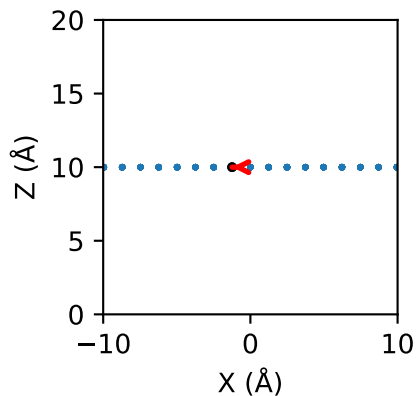
Distance = 5.748 Å  
 Cell vector (Rx, Ry, Rz) = (-1, -3, 0)  
 Cartesian vector (rx, ry, rz) = (0.0, -5.748, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



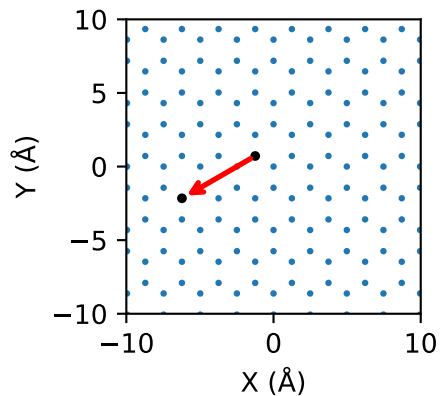
	pz
pz	-0.738



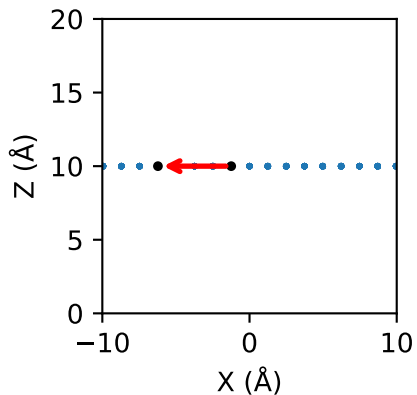
Distance = 5.748 Å  
 Cell vector (Rx, Ry, Rz) = (1, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-0.0, 5.748, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



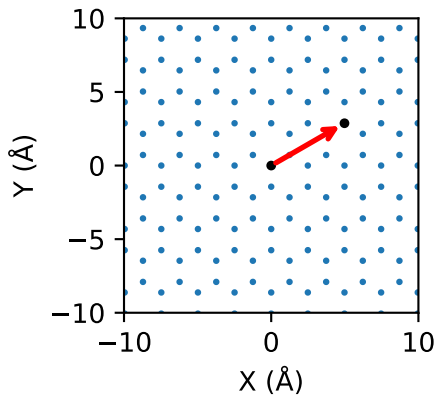
	pz
pz	-0.738



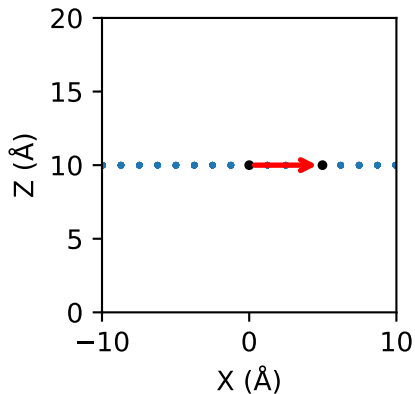
Distance = 5.748 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, -2.874, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-0.738

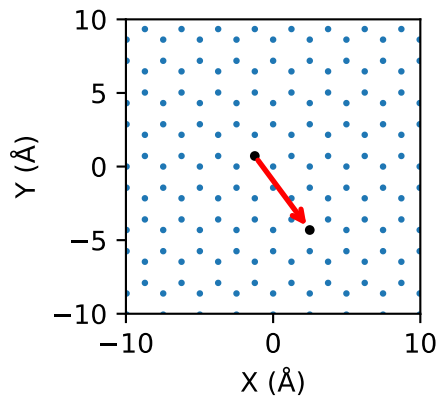


Distance = 5.748 Å  
 Cell vector (Rx, Ry, Rz) = (3, 1, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 2.874, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

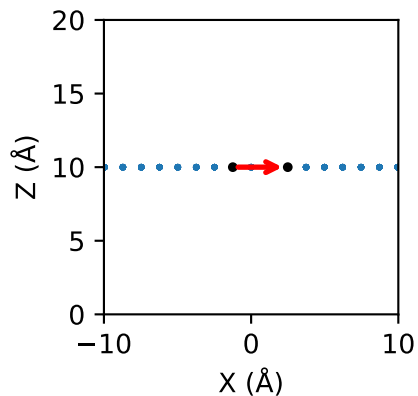


	pz
pz	-0.738

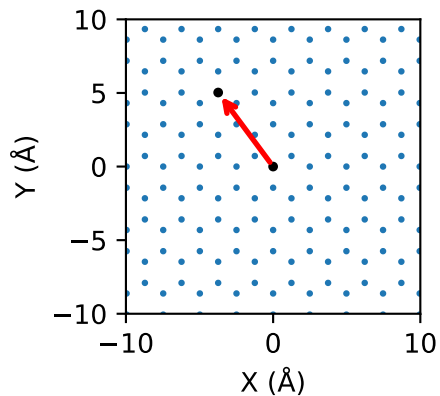




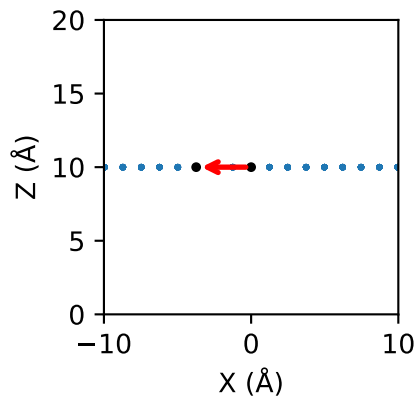
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (0, -2, 0)  
 Cartesian vector (rx, ry, rz) = (3.733, -5.03, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



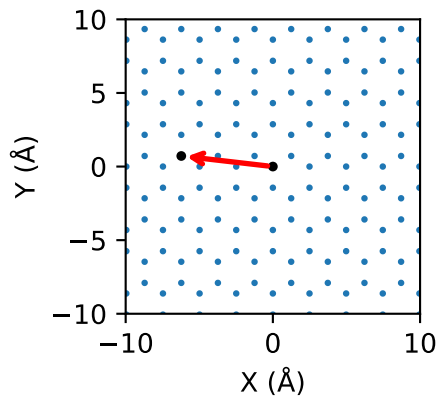
	pz
pz	11.606



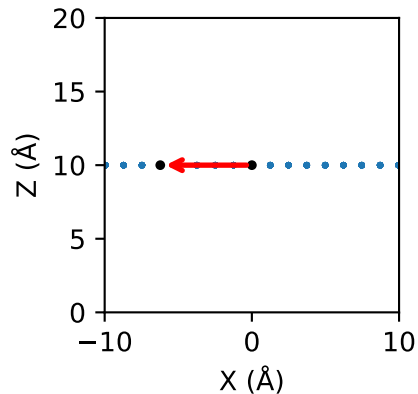
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (0, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-3.733, 5.03, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



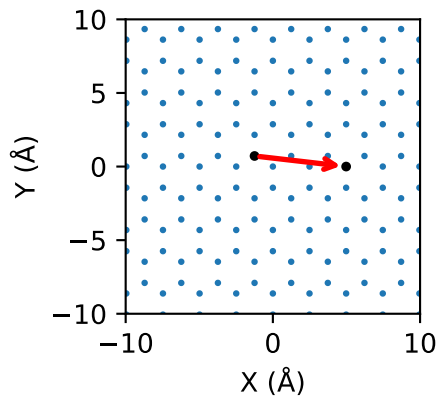
	pz
pz	11.606



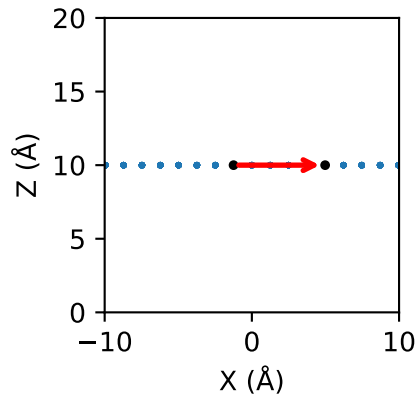
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-6.222, 0.718, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



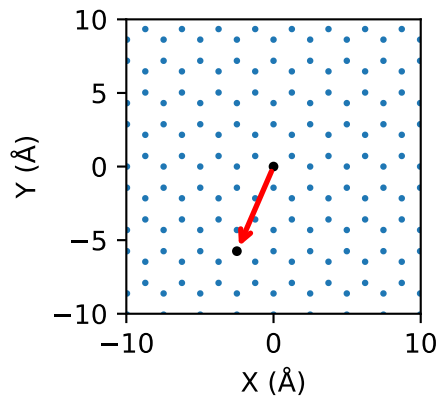
	pz
pz	11.588



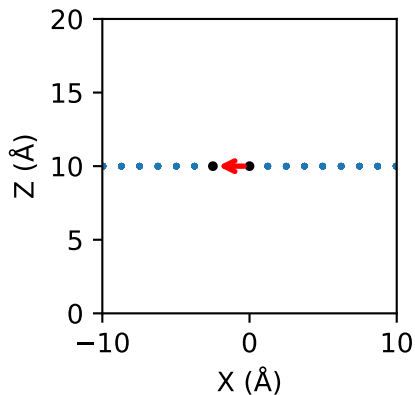
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (2, 0, 0)  
 Cartesian vector (rx, ry, rz) = (6.222, -0.718, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



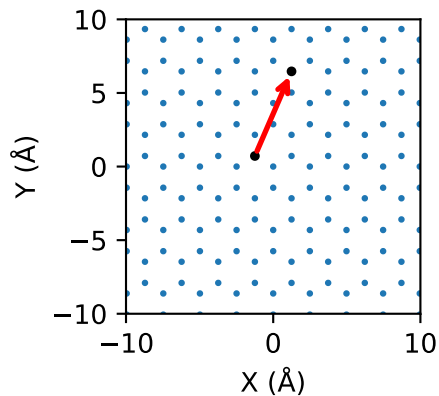
	pz
pz	11.588



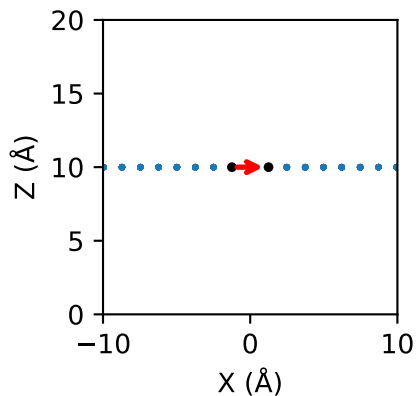
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, -5.748, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



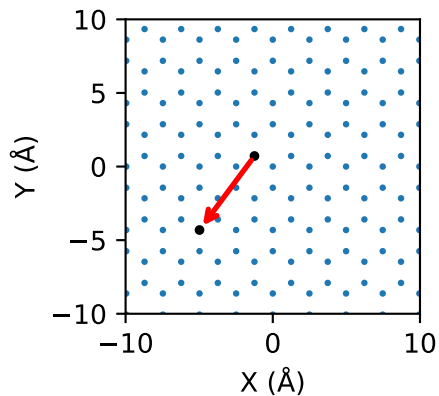
	pz
pz	-2.547



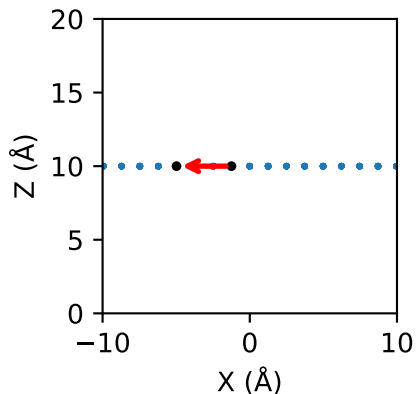
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (2, 3, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 5.748, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



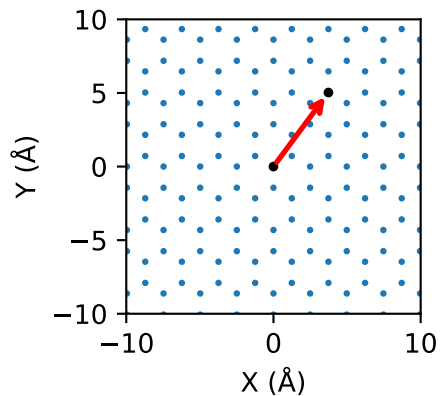
	pz
pz	-2.547



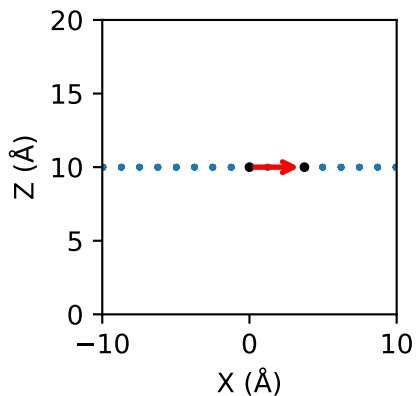
Distance = 6.264 Å  
 Cell vector ( $R_x, R_y, R_z$ ) = (-3, -2, 0)  
 Cartesian vector ( $r_x, r_y, r_z$ ) = (-3.734, -5.03, 0.0)  
 Atomic index ( $A_1, A_2$ ) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-2.547

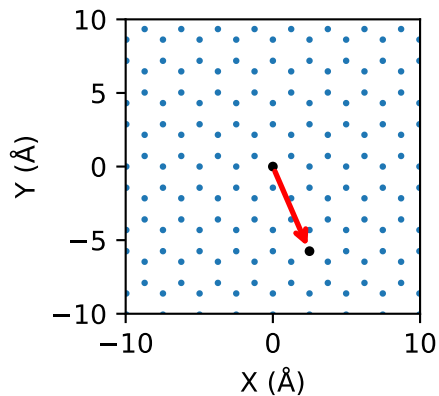


Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (3, 2, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, 5.03, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

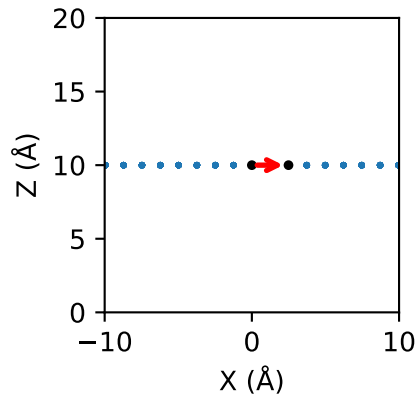


	pz
pz	-2.547

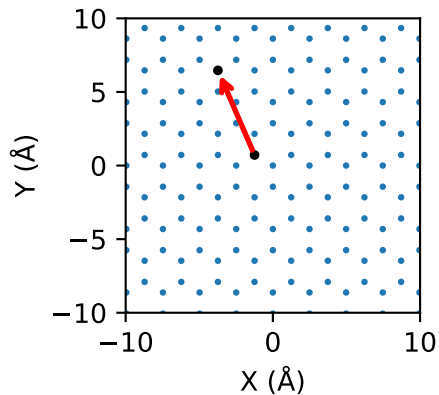




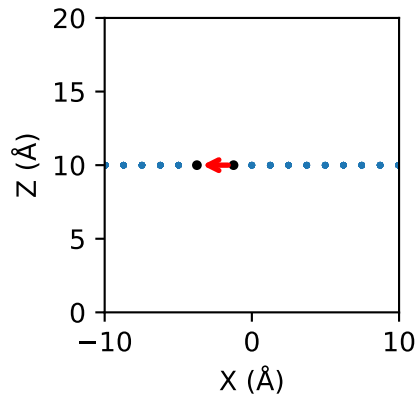
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (0, -3, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, -5.748, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



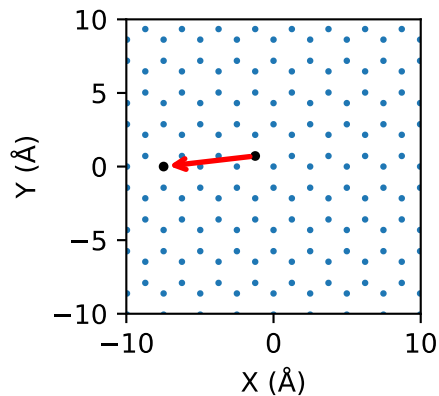
	pz
pz	0.326



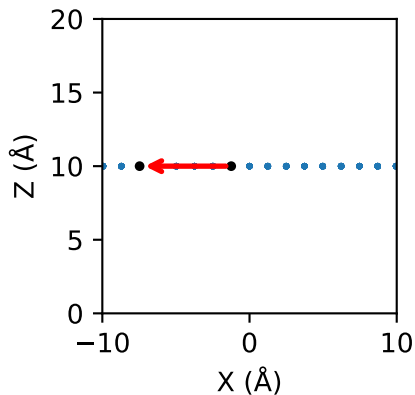
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (0, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 5.748, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



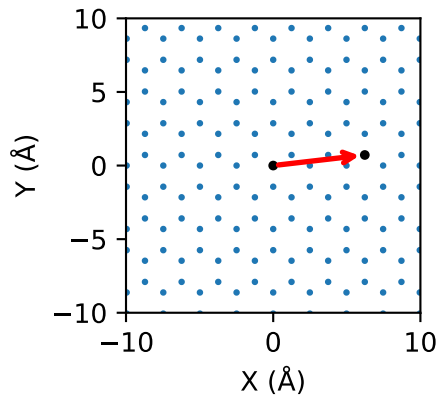
	pz
pz	0.326



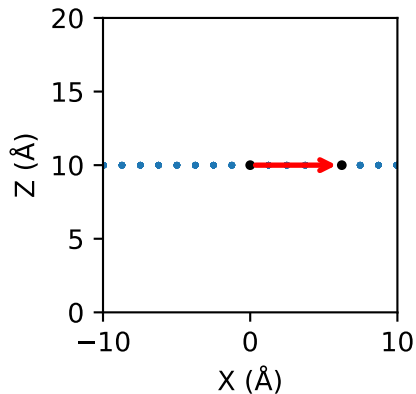
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (-3, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, -0.718, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



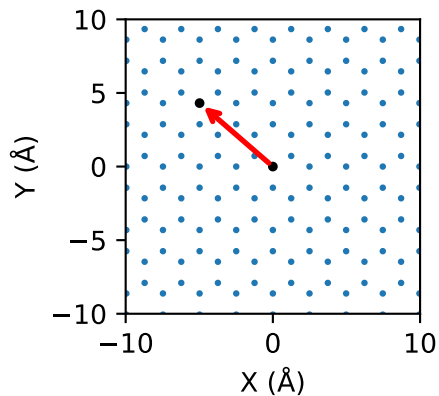
	pz
pz	0.327



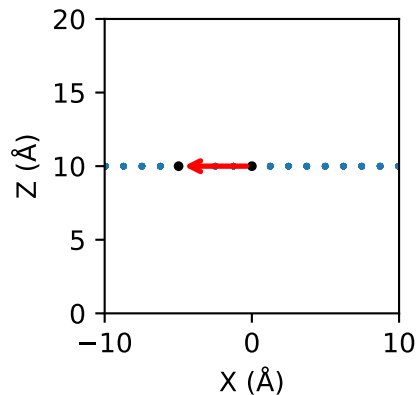
Distance = 6.264 Å  
 Cell vector (Rx, Ry, Rz) = (3, 0, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, 0.718, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



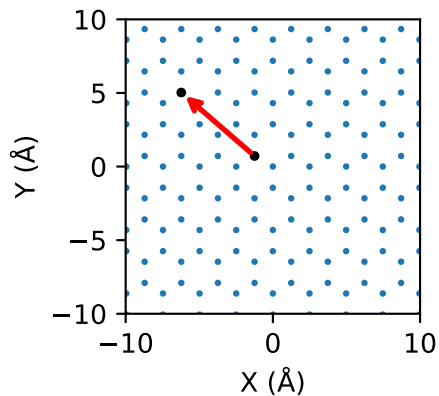
	pz
pz	0.327



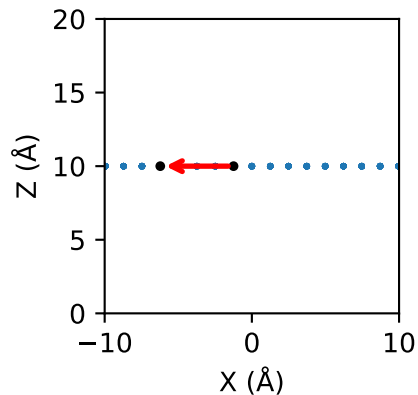
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



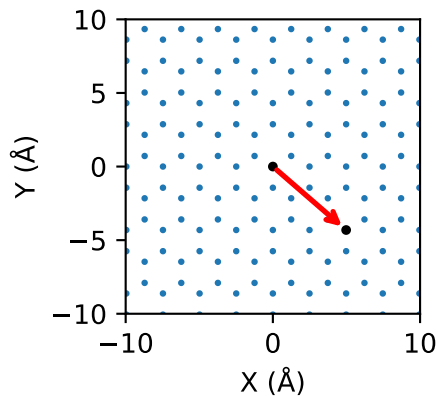
	pz
pz	4.32



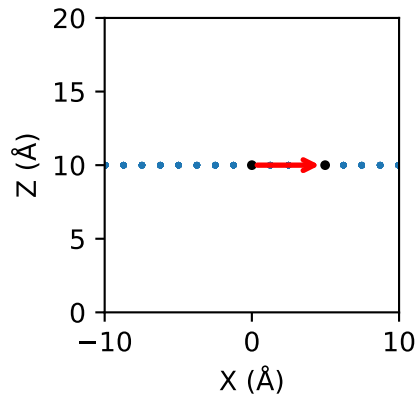
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



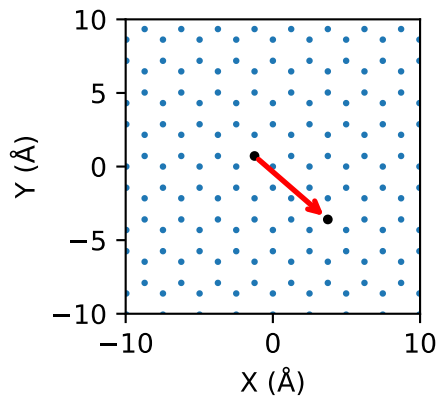
	pz
pz	4.32



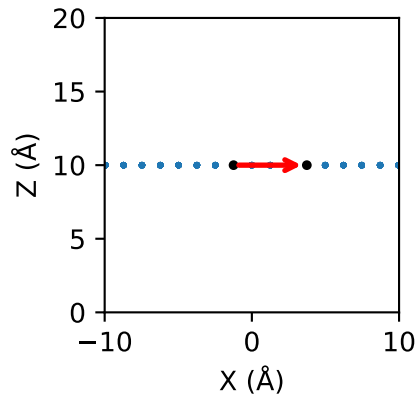
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (1, -2, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, -4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	4.32

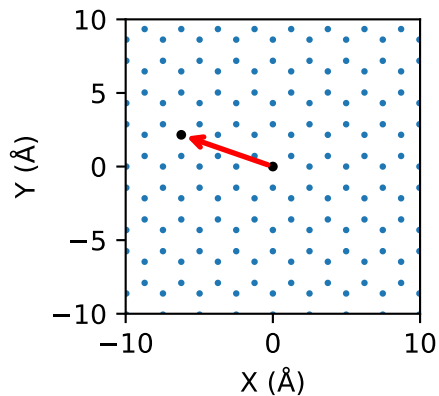


Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (1, -2, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, -4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

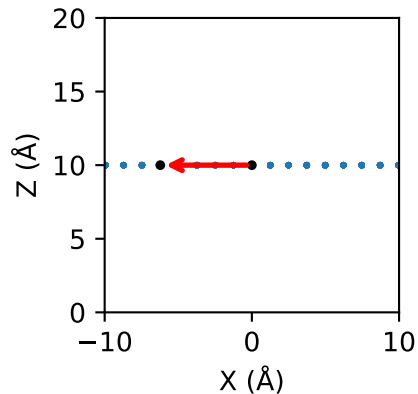


	pz
pz	4.32

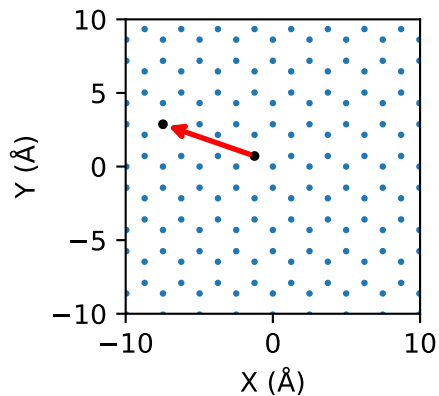




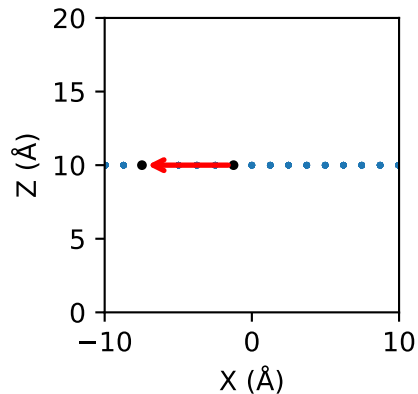
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, 2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



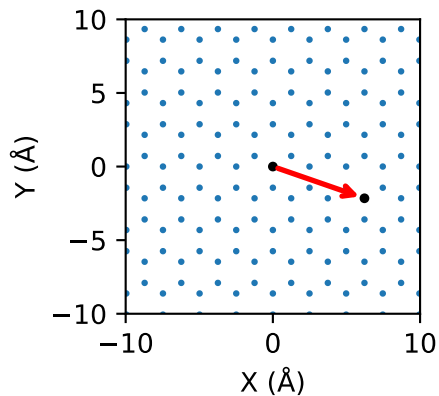
	pz
pz	4.322



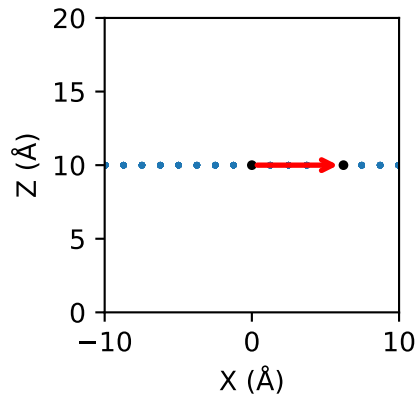
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, 2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



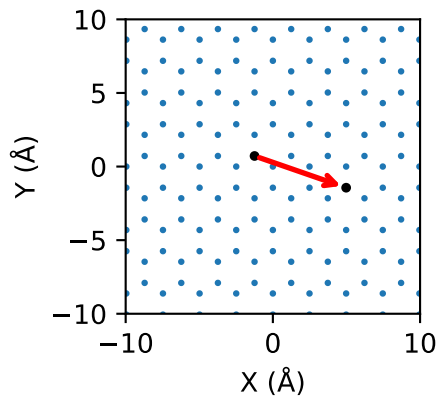
	pz
pz	4.322



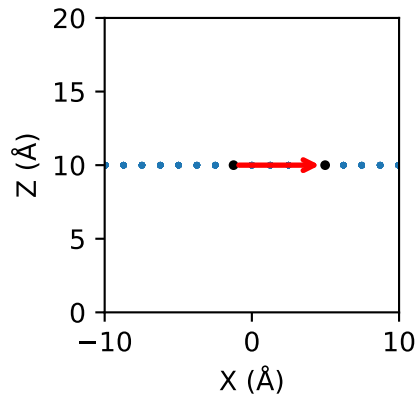
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (2, -1, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, -2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



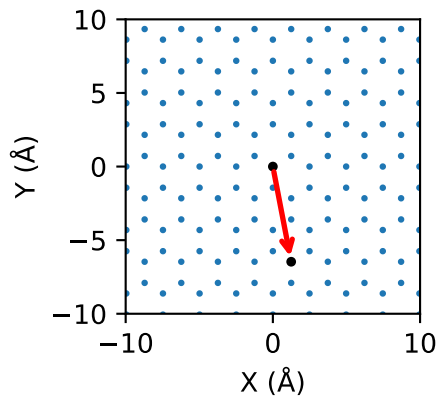
	pz
pz	4.322



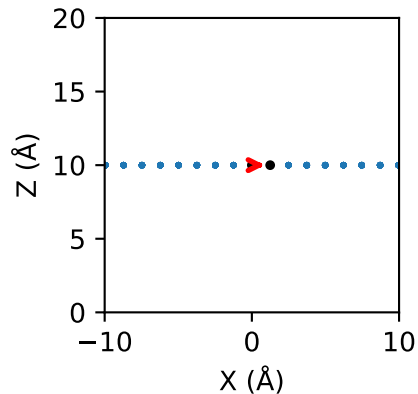
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (2, -1, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, -2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



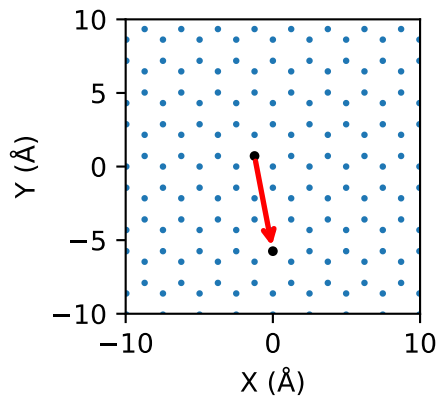
	pz
pz	4.322



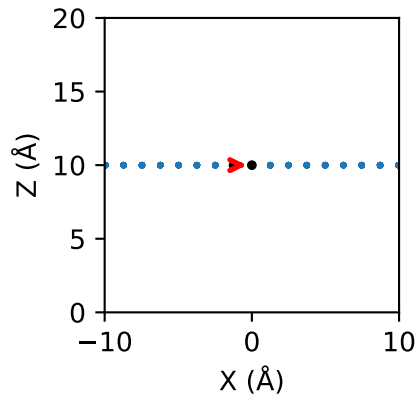
Distance = 6.585 Å  
 Cell vector ( $R_x, R_y, R_z$ ) = (-1, -3, 0)  
 Cartesian vector ( $r_x, r_y, r_z$ ) = (1.245, -6.467, 0.0)  
 Atomic index ( $A_1, A_2$ ) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



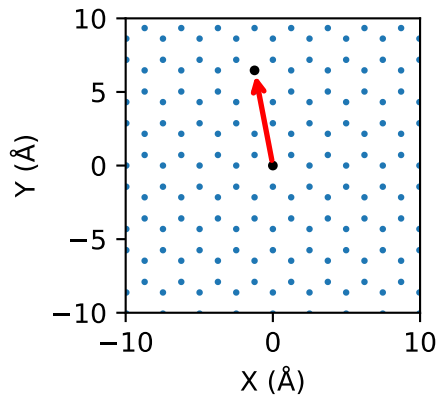
	pz
pz	4.32



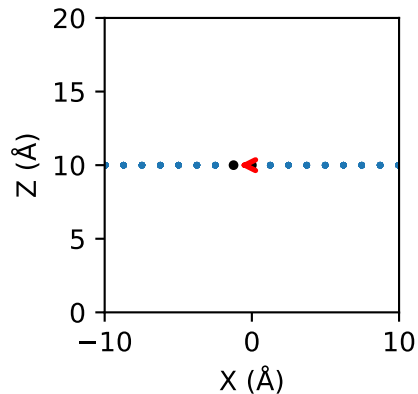
Distance = 6.585 Å  
 Cell vector ( $R_x, R_y, R_z$ ) = (-1, -3, 0)  
 Cartesian vector ( $r_x, r_y, r_z$ ) = (1.245, -6.467, 0.0)  
 Atomic index ( $A_1, A_2$ ) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



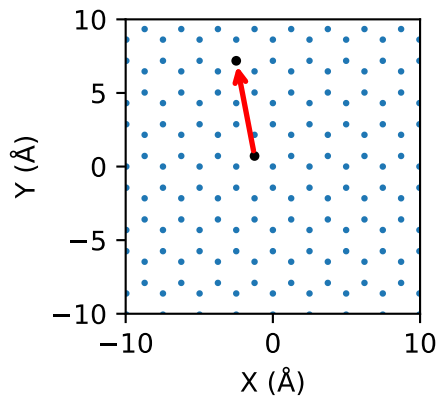
	pz
pz	4.32



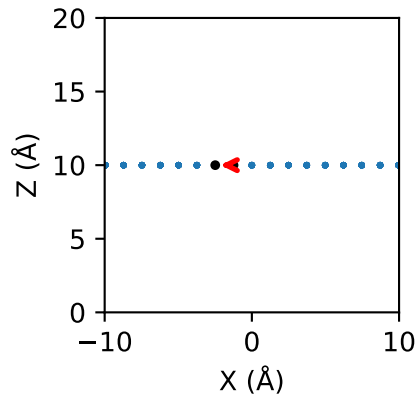
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (1, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, 6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	4.32

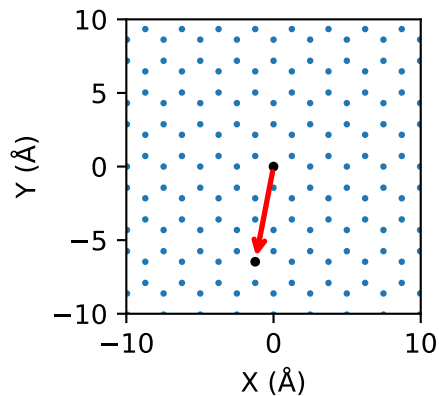


Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (1, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, 6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

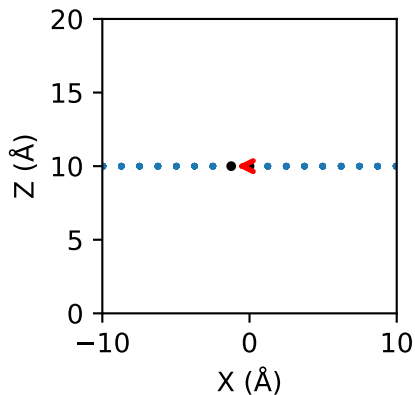


	pz
pz	4.32

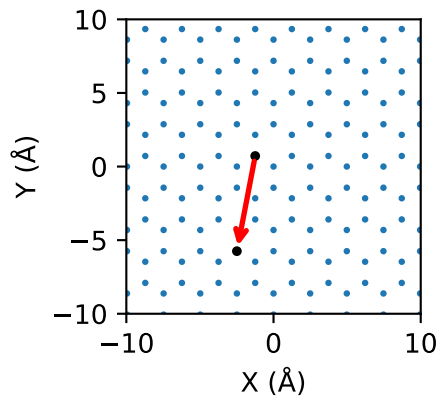




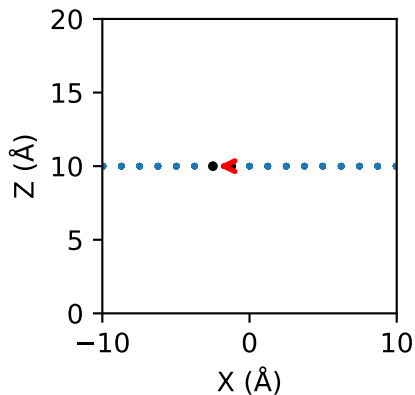
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, -6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



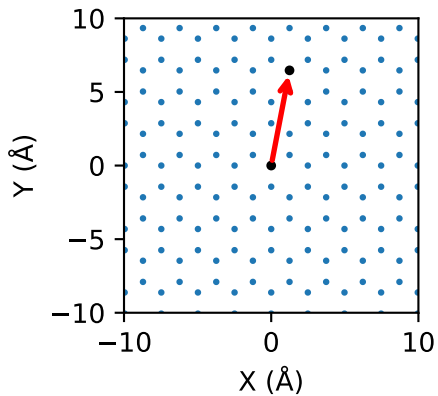
	pz
pz	4.318



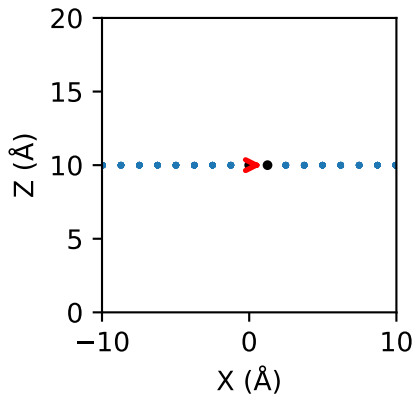
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, -6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



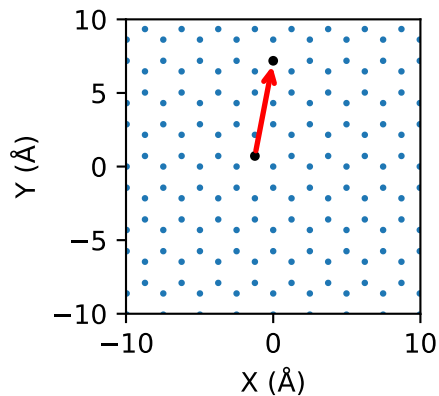
	pz
pz	4.318



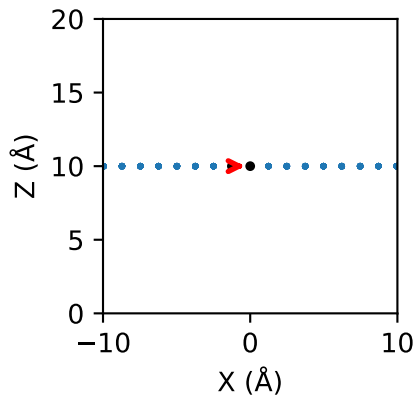
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (2, 3, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, 6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



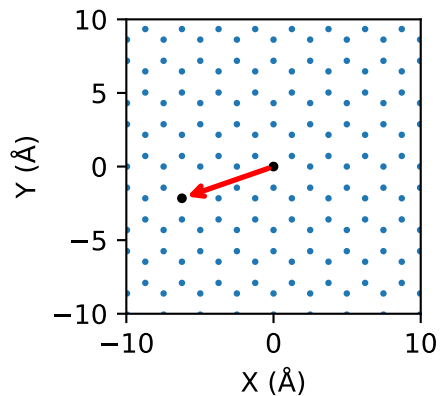
	pz
pz	4.318



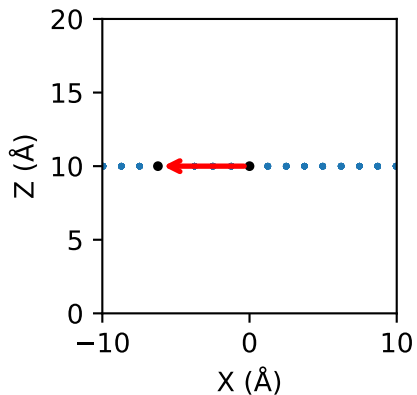
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (2, 3, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, 6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



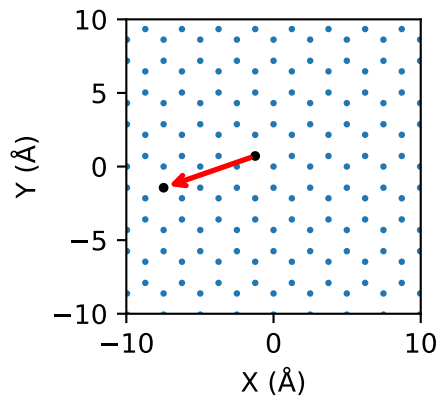
	pz
pz	4.318



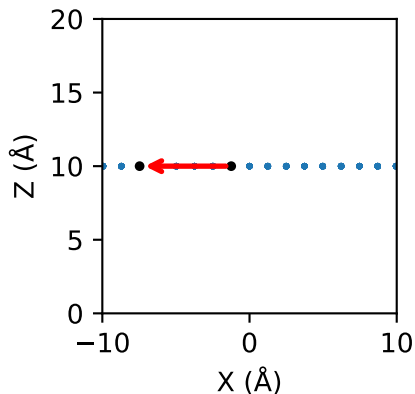
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, -2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



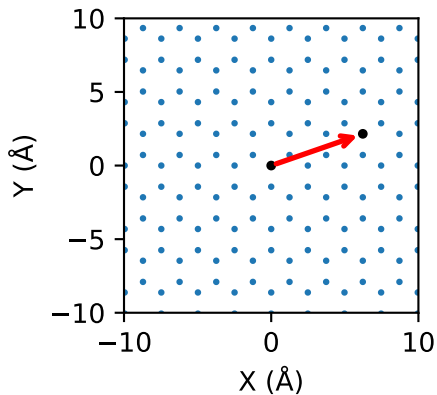
	pz
pz	4.322



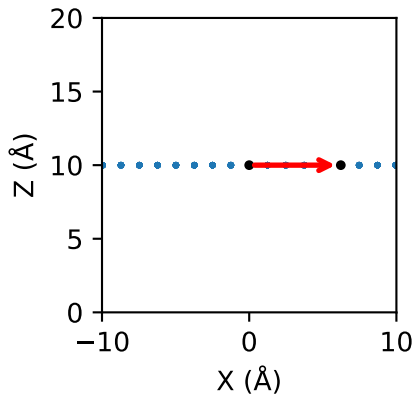
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, -2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



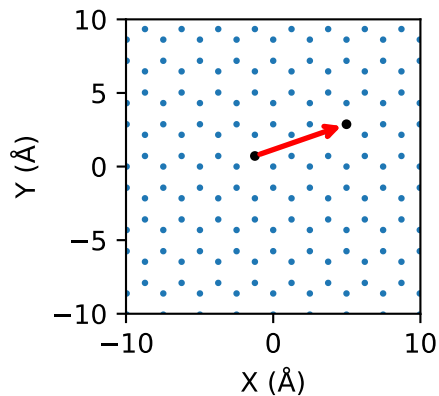
	pz
pz	4.322



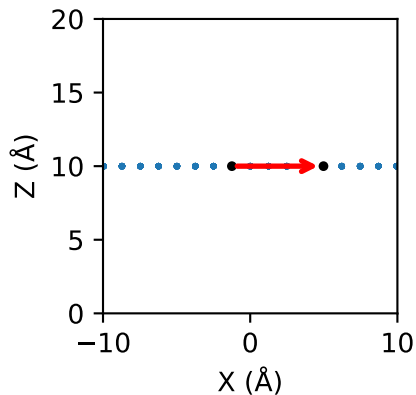
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (3, 1, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, 2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	4.322

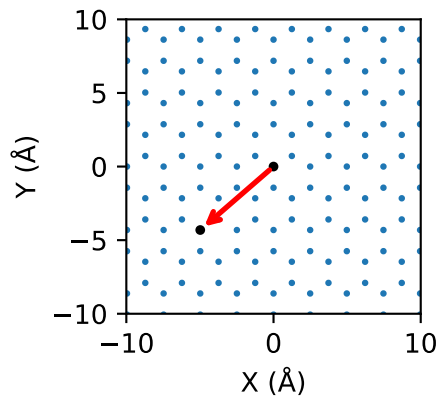


Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (3, 1, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, 2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

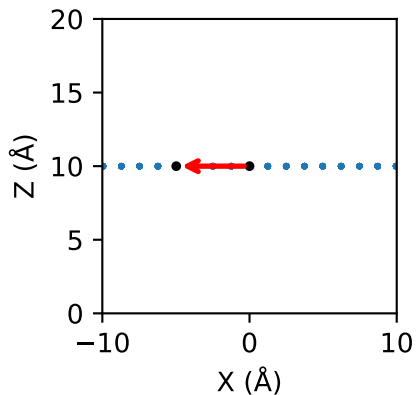


	pz
pz	4.322

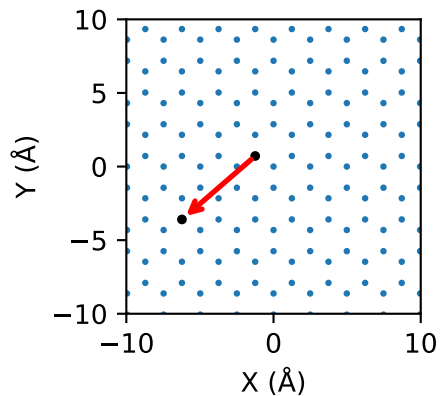




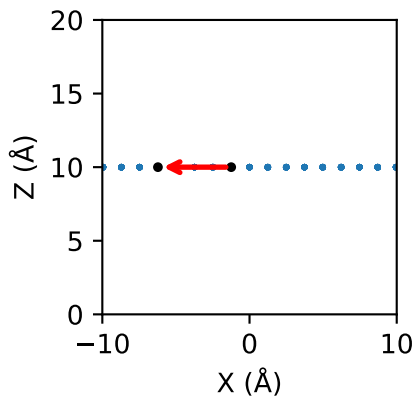
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, -4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



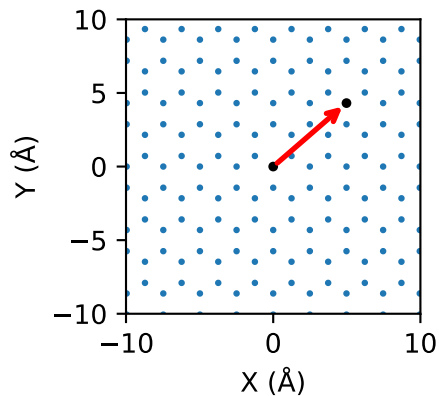
	pz
pz	4.318



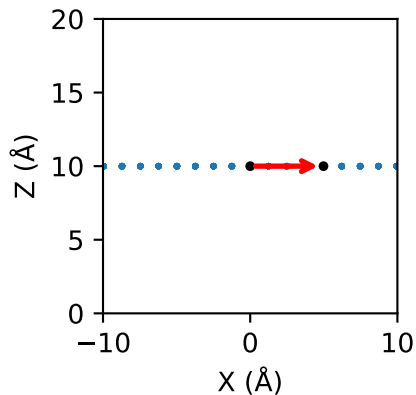
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, -4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



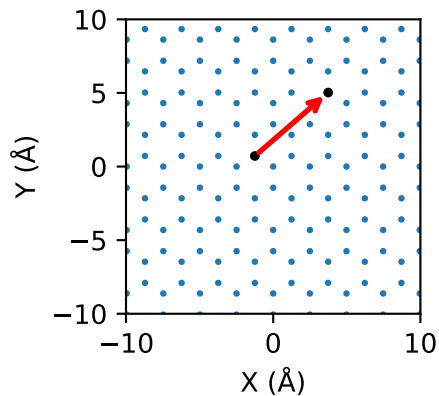
	pz
pz	4.318



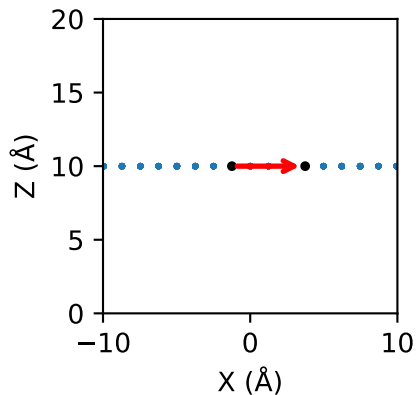
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (3, 2, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



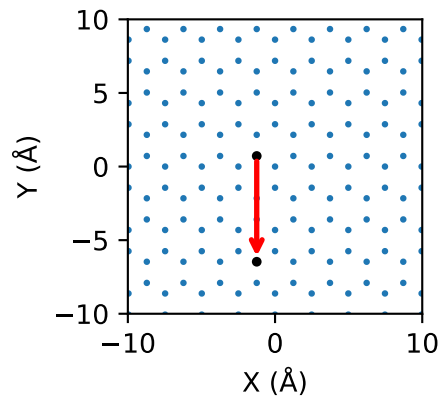
	pz
pz	4.318



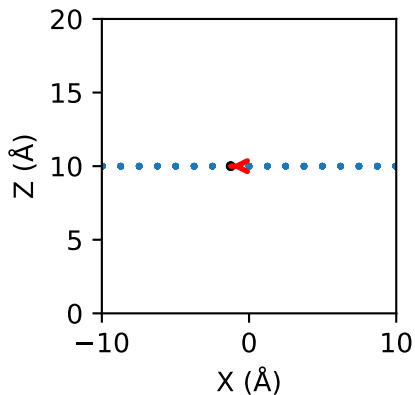
Distance = 6.585 Å  
 Cell vector (Rx, Ry, Rz) = (3, 2, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



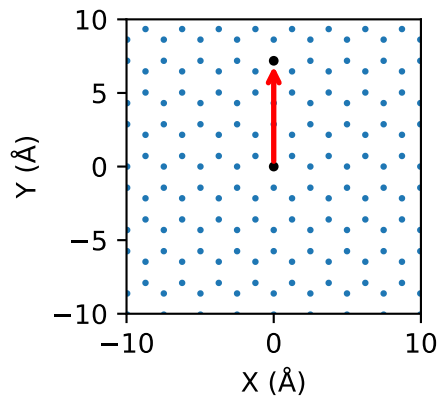
	pz
pz	4.318



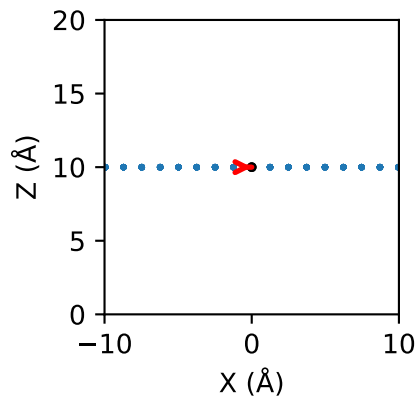
Distance = 7.185 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-0.0, -7.185, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



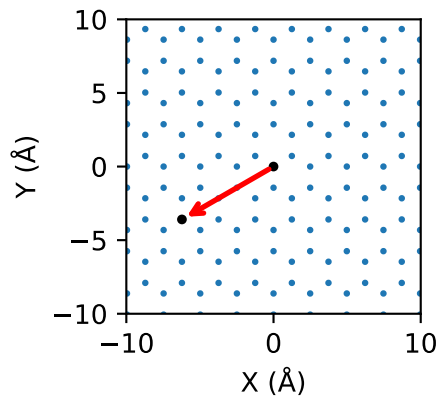
	pz
pz	6.171



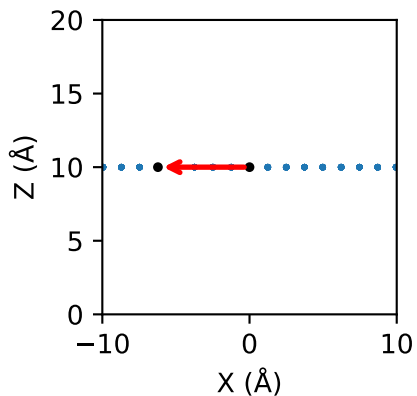
Distance = 7.185 Å  
 Cell vector (Rx, Ry, Rz) = (2, 3, 0)  
 Cartesian vector (rx, ry, rz) = (0.0, 7.185, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



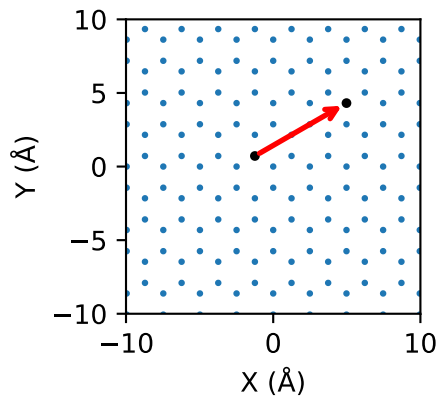
	pz
pz	6.171



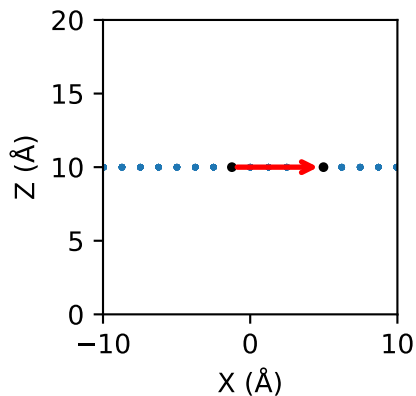
Distance = 7.185 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-6.222, -3.593, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



	pz
pz	6.171

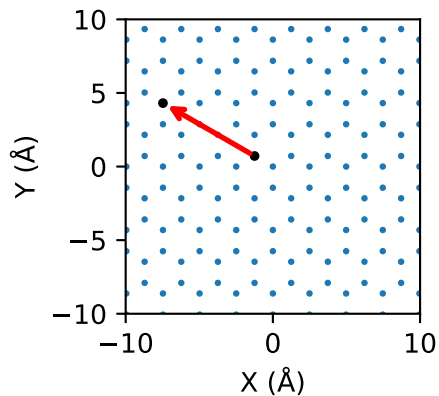


Distance = 7.185 Å  
 Cell vector (Rx, Ry, Rz) = (3, 2, 0)  
 Cartesian vector (rx, ry, rz) = (6.222, 3.593, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV

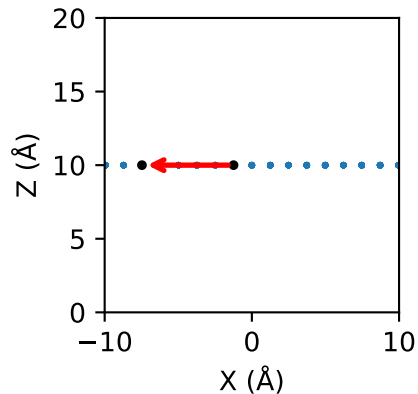


	pz
pz	6.171

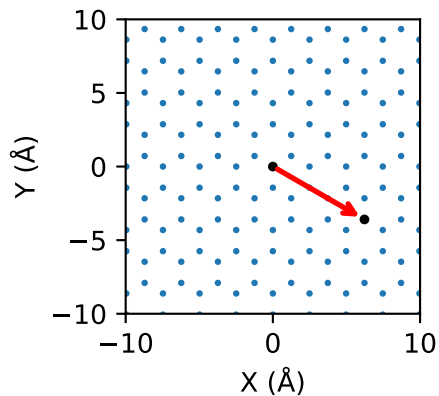




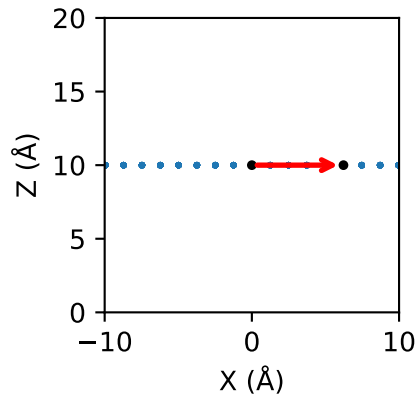
Distance = 7.185 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, 3.593, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



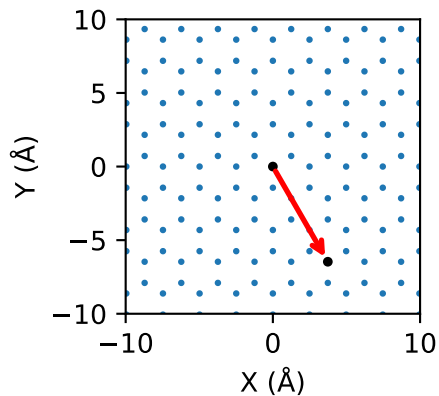
	pz
pz	-0.478



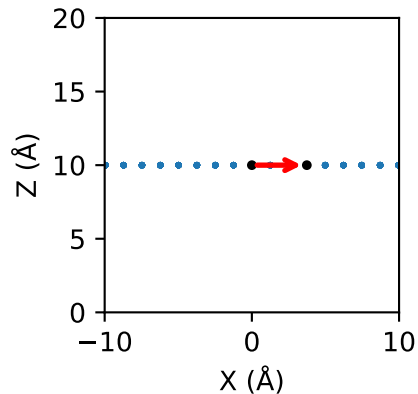
Distance = 7.185 Å  
 Cell vector (Rx, Ry, Rz) = (2, -2, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, -3.593, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



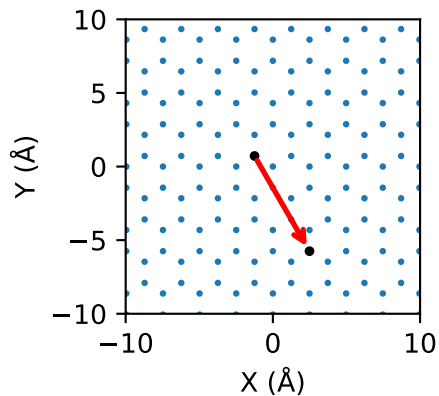
	pz
pz	-0.478



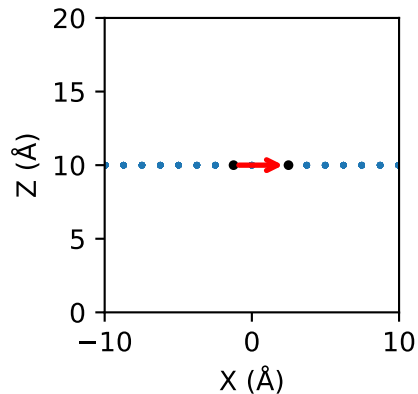
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (0, -3, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, -6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



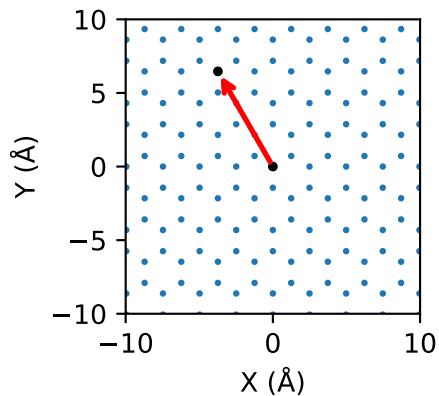
	pz
pz	-1.821



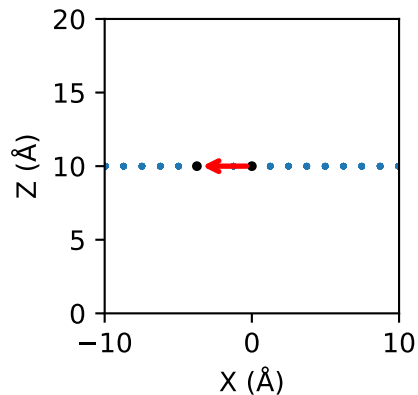
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (0, -3, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, -6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



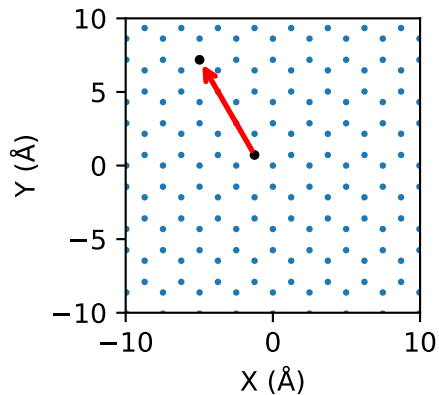
	pz
pz	-1.821



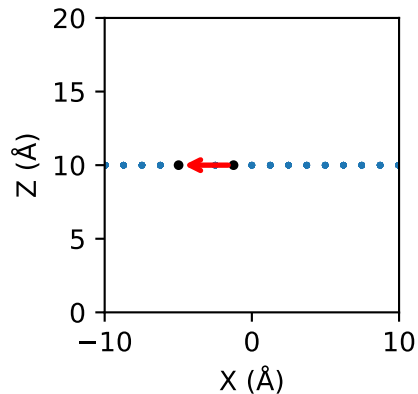
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (0, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, 6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



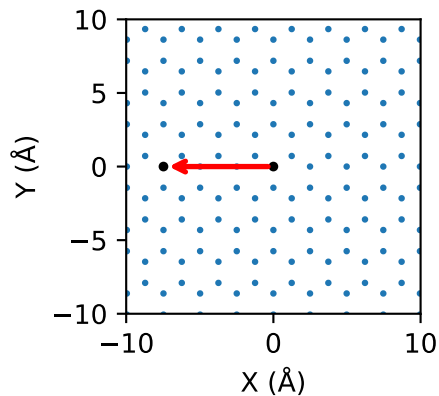
	pz
pz	-1.821



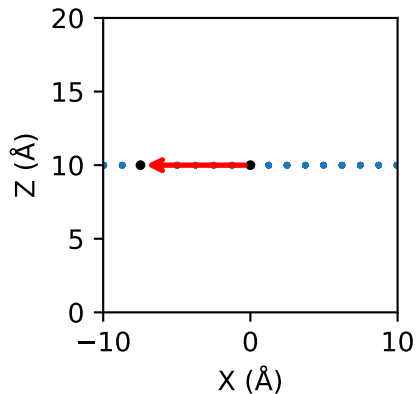
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (0, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, 6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



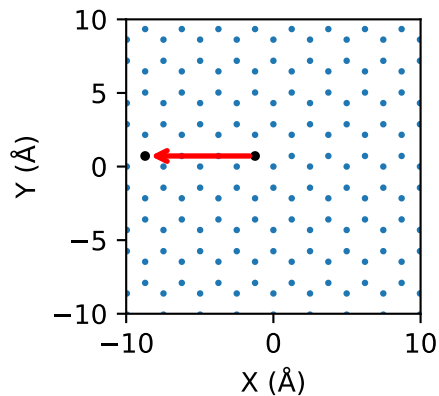
	pz
pz	-1.821



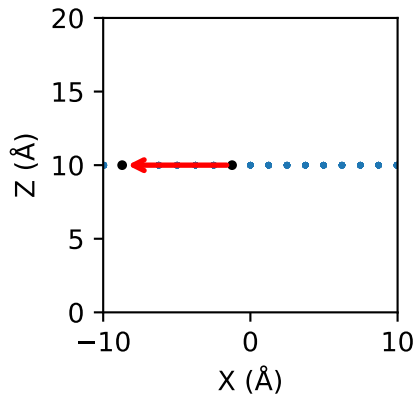
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (-3, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, 0.0, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-1.822

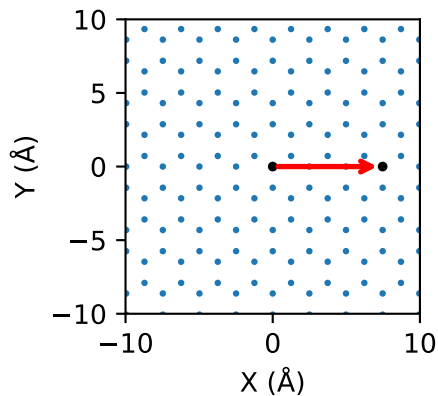


Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (-3, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, 0.0, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

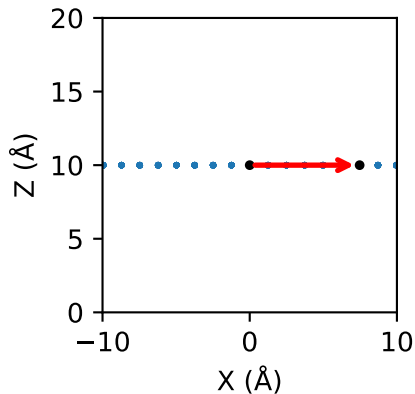


	pz
pz	-1.822

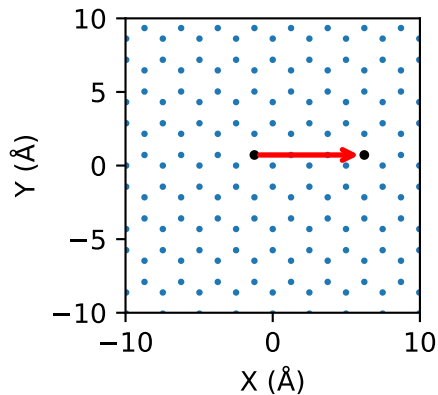




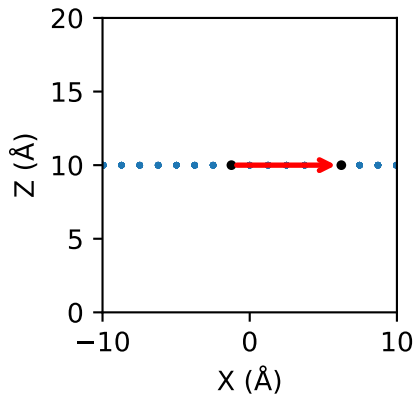
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (3, 0, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, 0.0, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



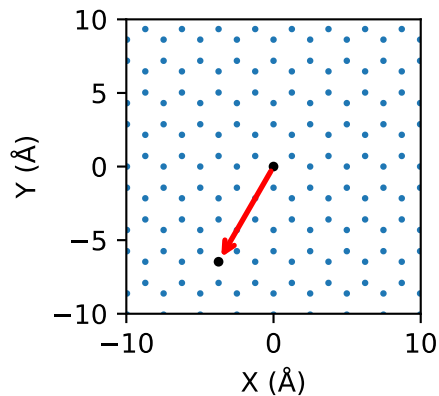
	pz
pz	-1.822



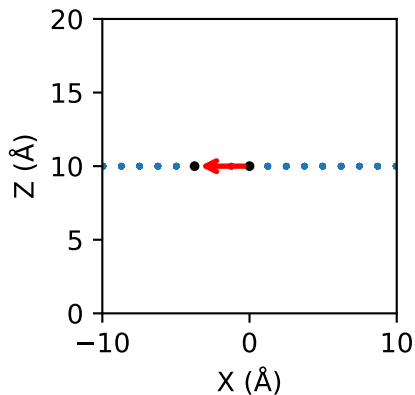
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (3, 0, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, 0.0, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



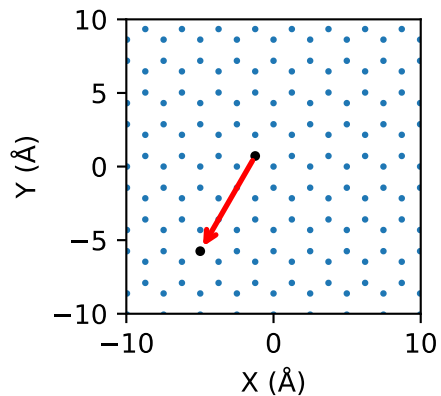
	pz
pz	-1.822



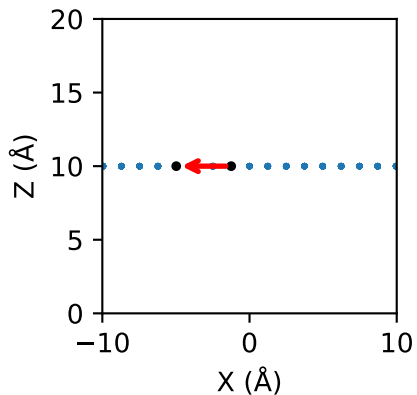
Distance = 7.467 Å  
 Cell vector ( $R_x$ ,  $R_y$ ,  $R_z$ ) = (-3, -3, 0)  
 Cartesian vector ( $r_x$ ,  $r_y$ ,  $r_z$ ) = (-3.734, -6.467, 0.0)  
 Atomic index ( $A_1$ ,  $A_2$ ) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



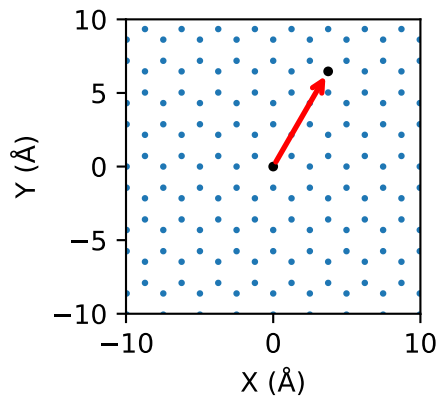
	pz
pz	-1.82



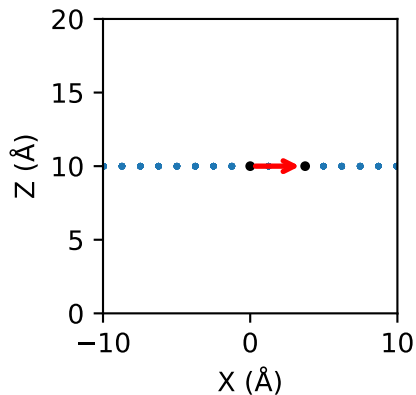
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, -6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



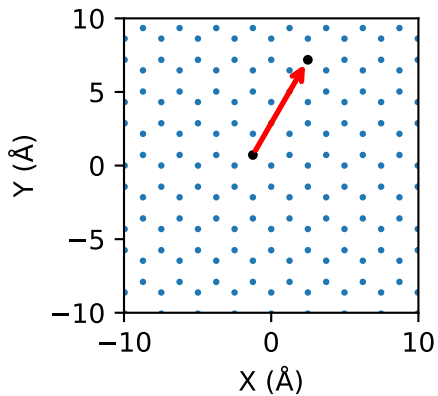
	pz
pz	-1.82



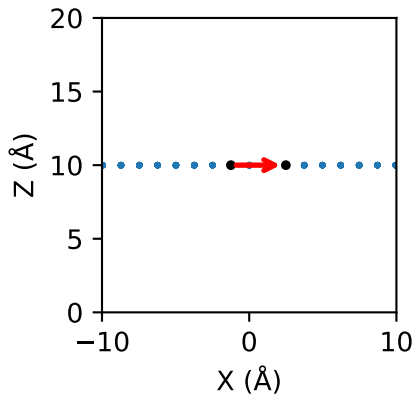
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (3, 3, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, 6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



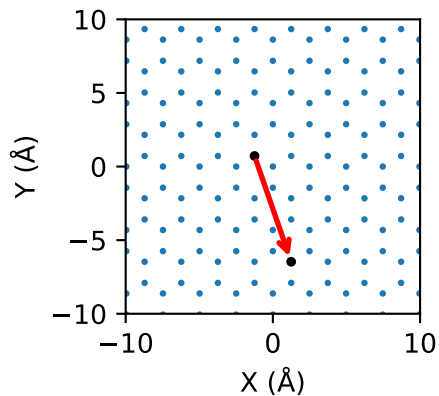
	pz
pz	-1.82



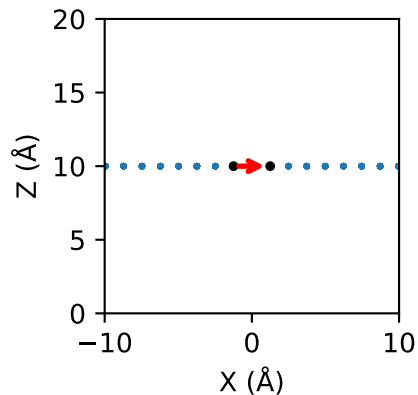
Distance = 7.467 Å  
 Cell vector (Rx, Ry, Rz) = (3, 3, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, 6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



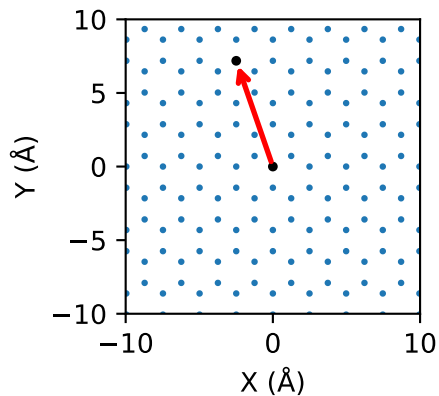
	pz
pz	-1.82



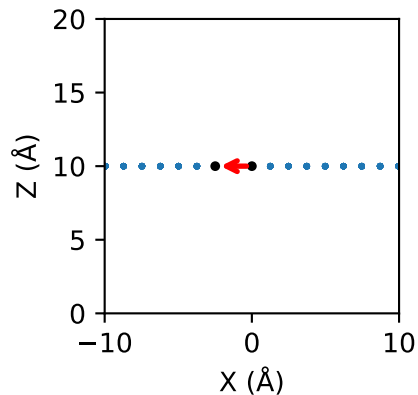
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (-1, -3, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, -7.185, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-22.269

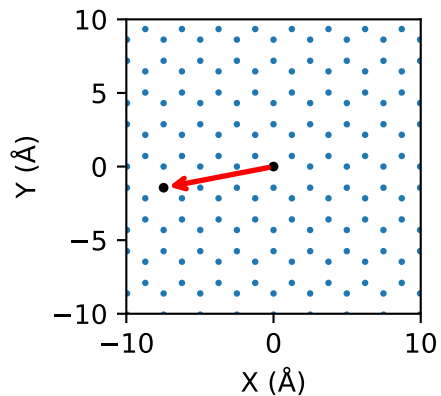


Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (1, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 7.185, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

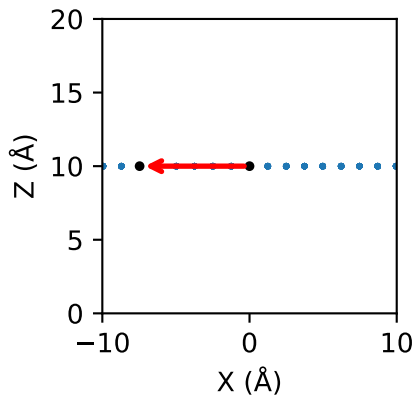


	pz
pz	-22.269

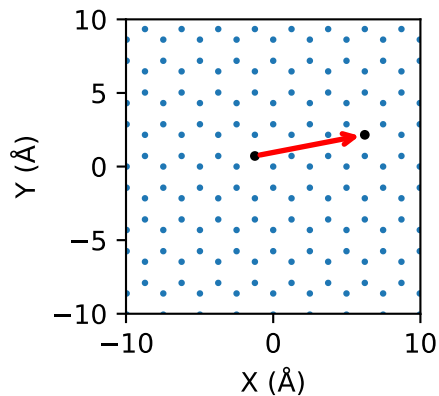




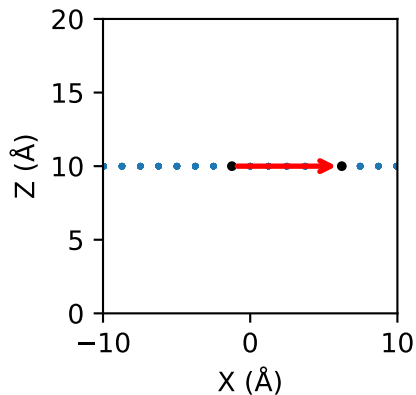
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, -1.437, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



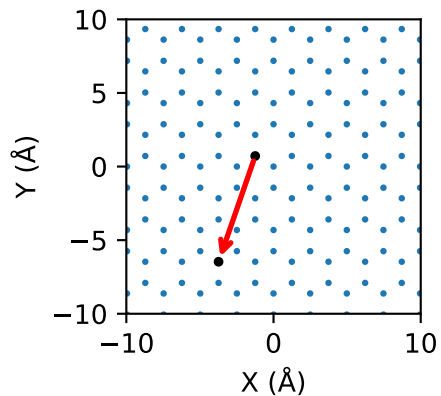
	pz
pz	-22.274



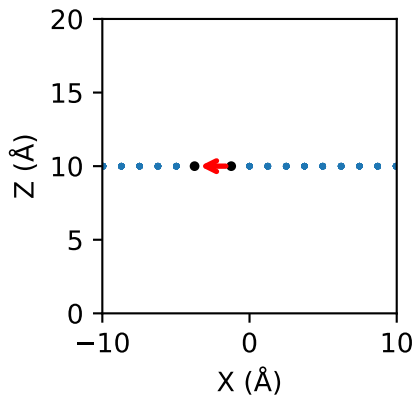
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (3, 1, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, 1.437, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



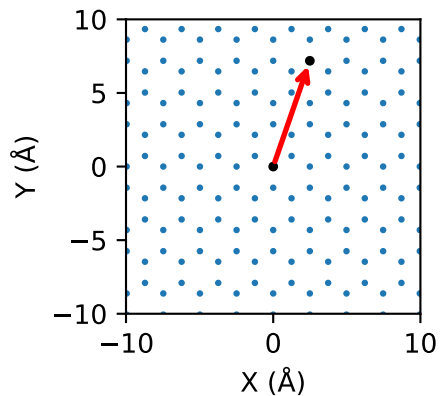
	pz
pz	-22.274



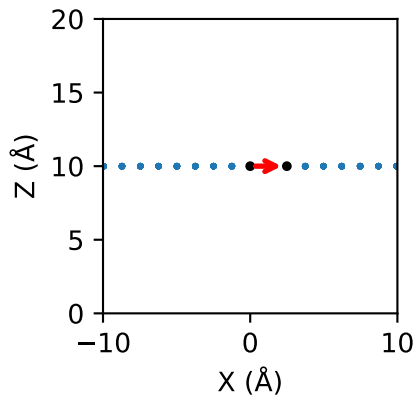
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, -7.185, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



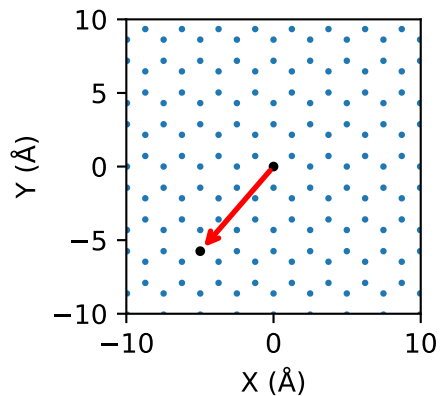
	pz
pz	-0.736



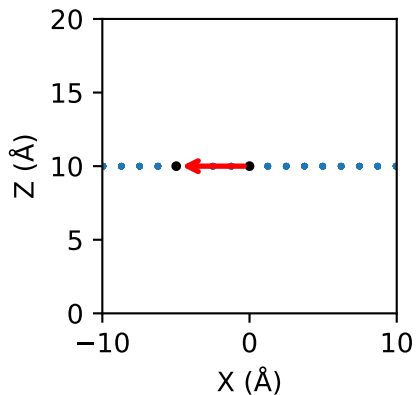
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (3, 3, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 7.185, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



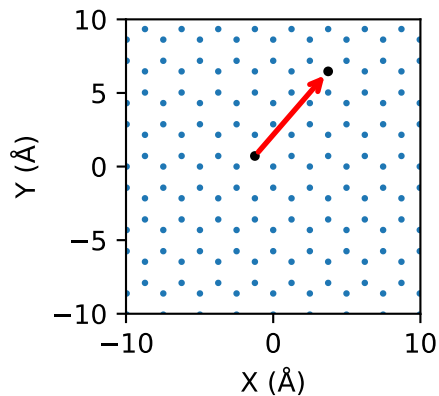
	pz
pz	-0.736



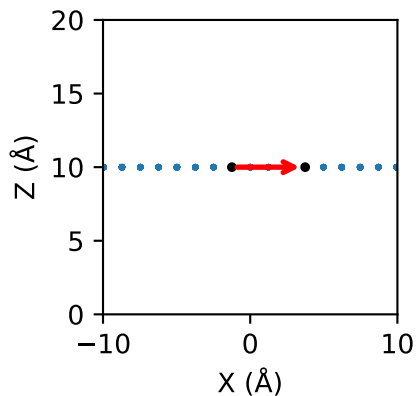
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, -5.748, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



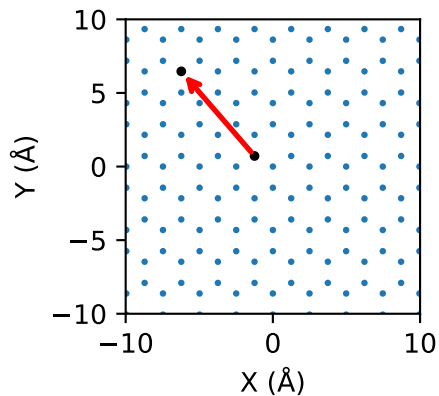
	pz
pz	-0.737



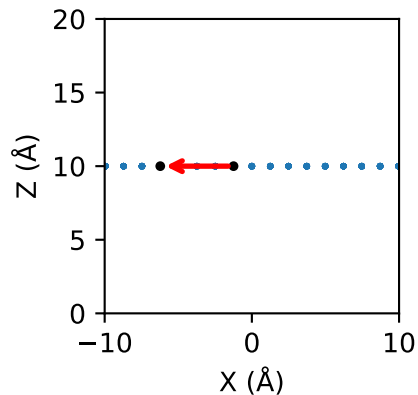
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (3, 3, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 5.748, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



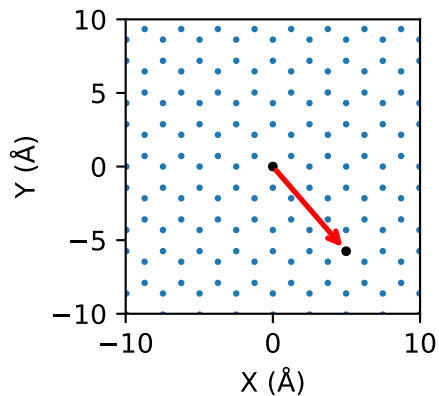
	pz
pz	-0.737



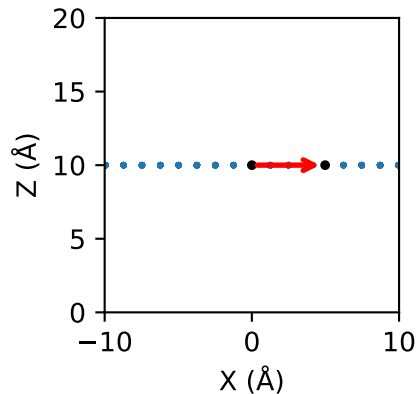
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 5.748, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-0.034

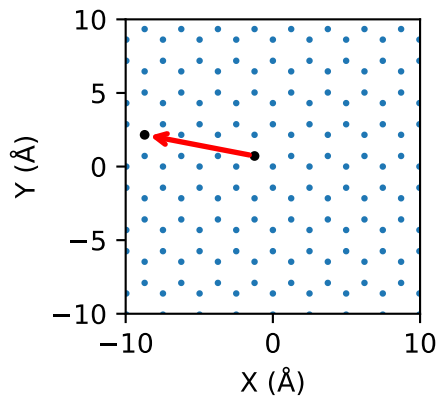


Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (1, -3, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, -5.748, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

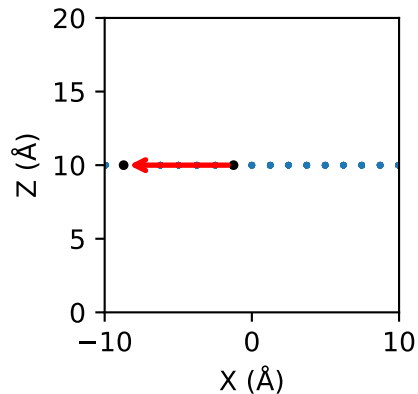


	pz
pz	-0.034

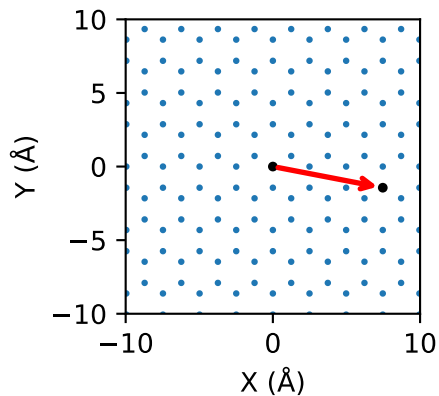




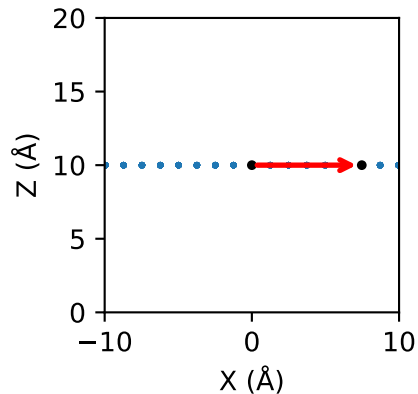
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (-3, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, 1.437, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



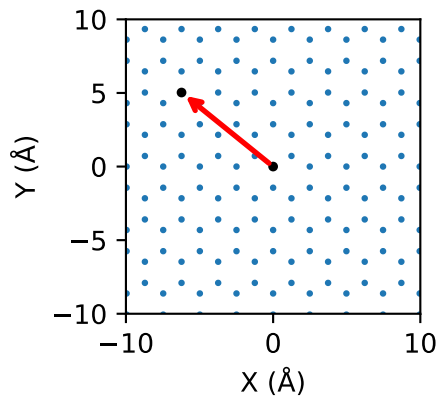
	pz
pz	-0.034



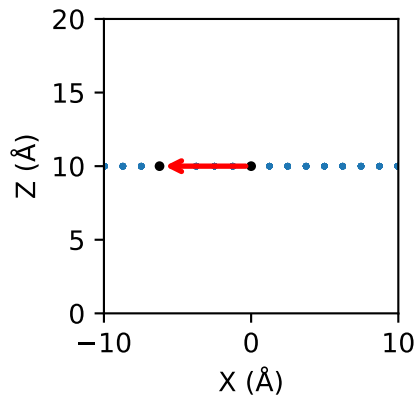
Distance = 7.604 Å  
 Cell vector (Rx, Ry, Rz) = (3, -1, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, -1.437, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



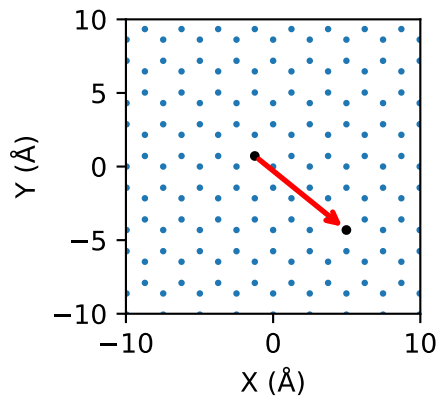
	pz
pz	-0.034



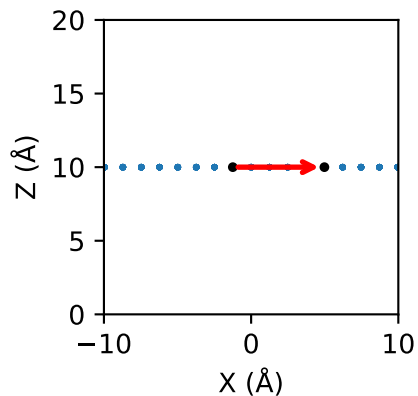
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-6.222, 5.03, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



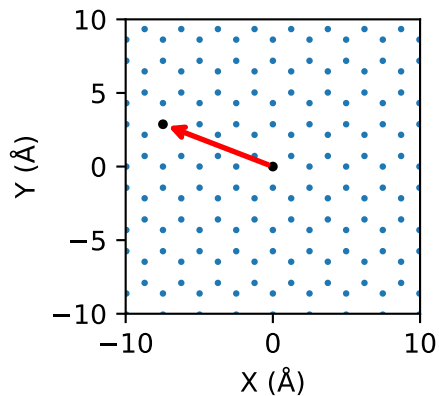
	pz
pz	-9.699



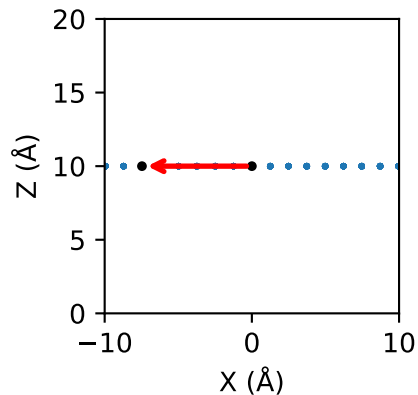
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (1, -2, 0)  
 Cartesian vector (rx, ry, rz) = (6.222, -5.03, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



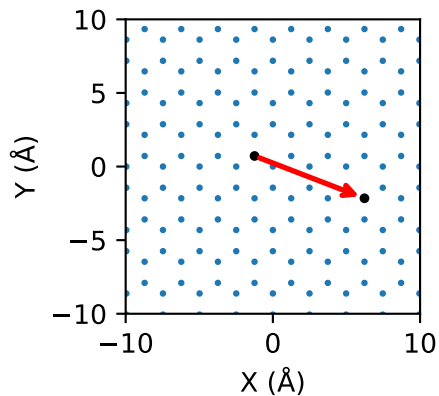
	pz
pz	-9.699



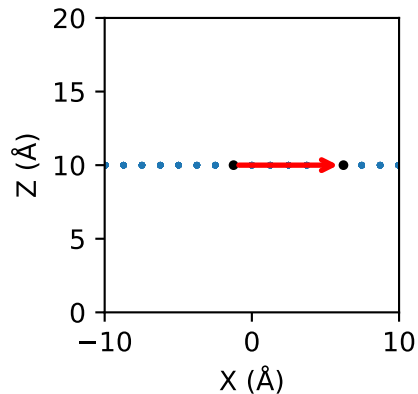
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, 2.874, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



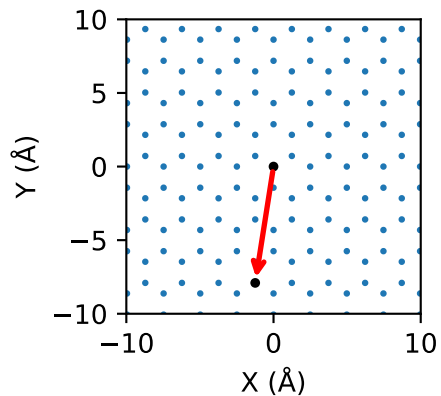
	pz
pz	-9.705



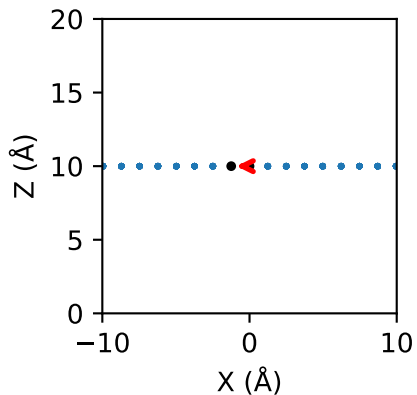
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (2, -1, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, -2.874, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



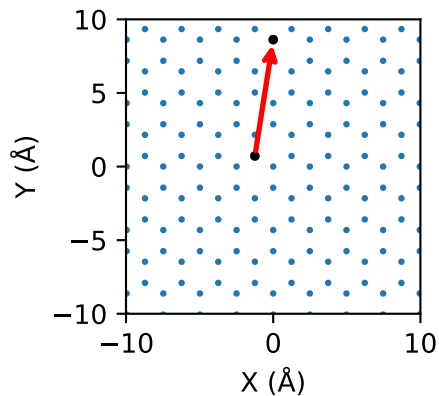
	pz
pz	-9.705



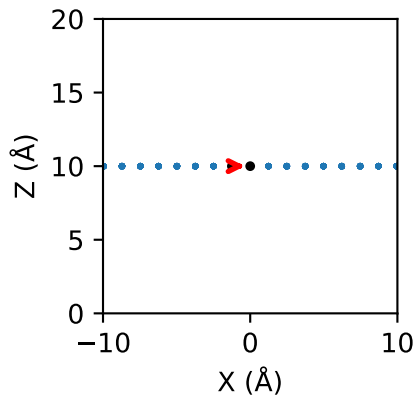
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-1.244, -7.904, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



	pz
pz	-0.338

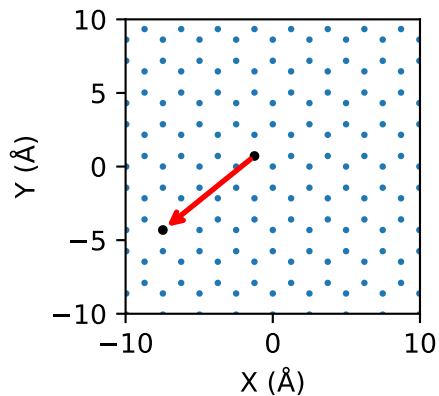


Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (2, 4, 0)  
 Cartesian vector (rx, ry, rz) = (1.244, 7.904, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV

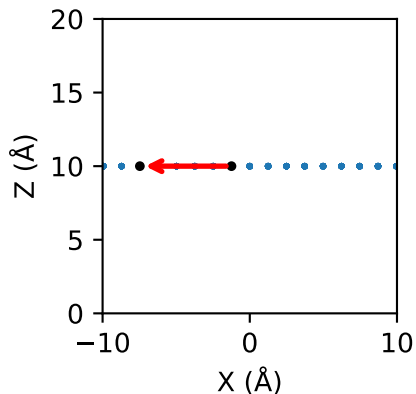


	pz
pz	-0.338

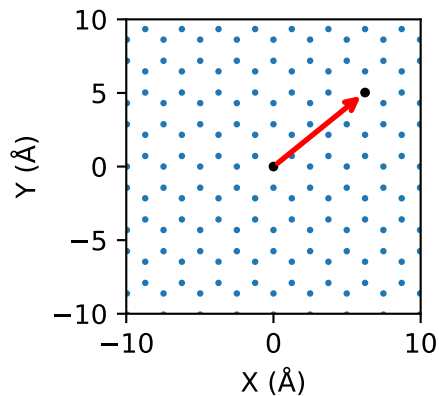




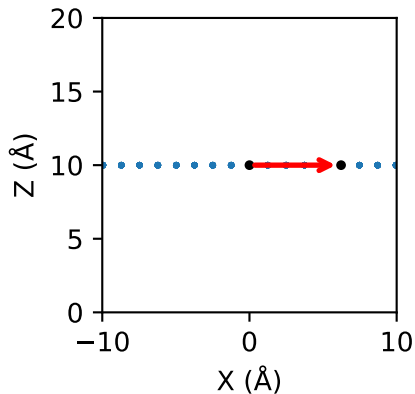
Distance = 8.001 Å  
 Cell vector ( $R_x, R_y, R_z$ ) = (-4, -2, 0)  
 Cartesian vector ( $r_x, r_y, r_z$ ) = (-6.223, -5.03, 0.0)  
 Atomic index ( $A_1, A_2$ ) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



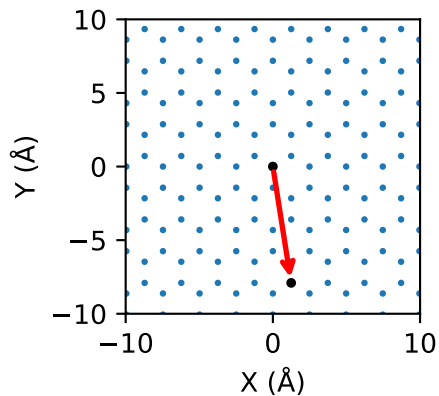
	pz
pz	-0.339



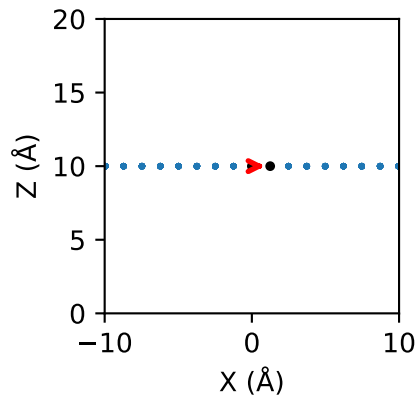
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (4, 2, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, 5.03, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



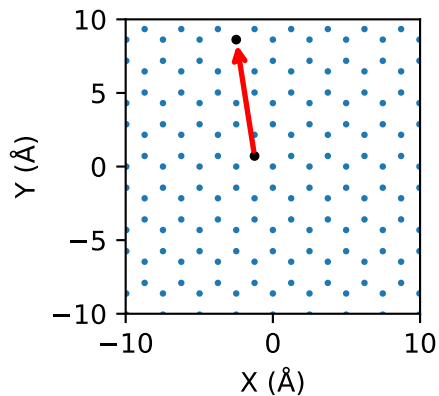
	pz
pz	-0.339



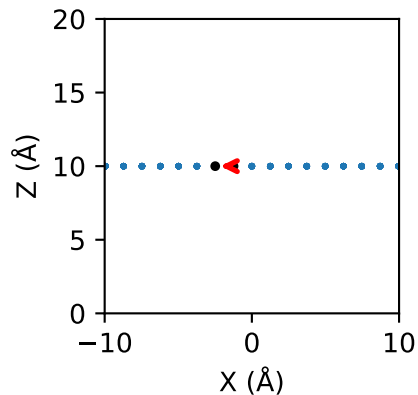
Distance = 8.001 Å  
 Cell vector ( $R_x, R_y, R_z$ ) = (-1, -4, 0)  
 Cartesian vector ( $r_x, r_y, r_z$ ) = (1.245, -7.904, 0.0)  
 Atomic index ( $A_1, A_2$ ) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



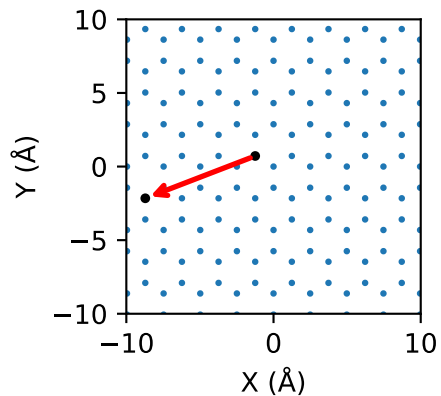
	pz
pz	0.517



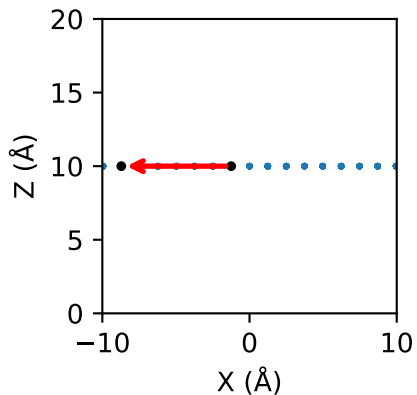
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (1, 4, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, 7.904, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



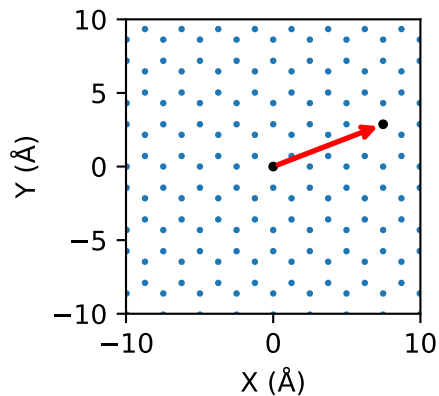
	pz
pz	0.517



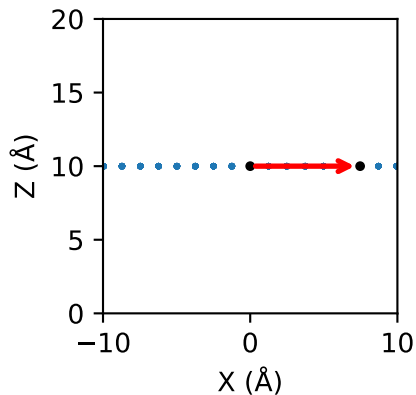
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, -2.874, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



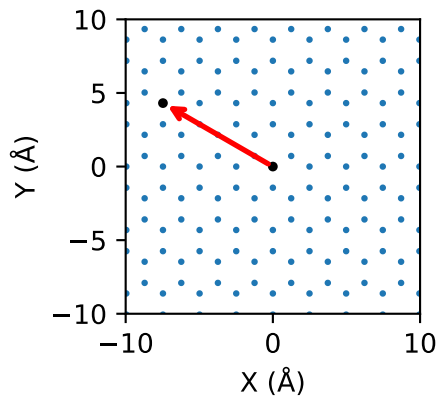
	pz
pz	0.517



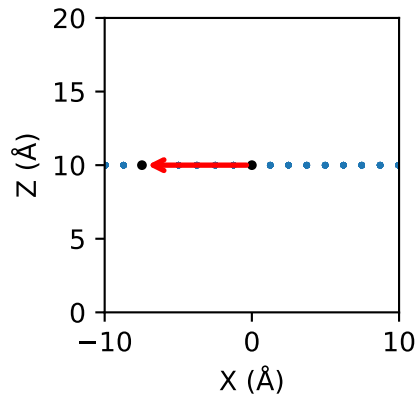
Distance = 8.001 Å  
 Cell vector (Rx, Ry, Rz) = (4, 1, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, 2.874, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



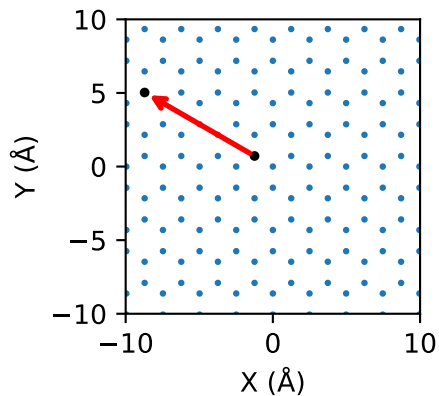
	pz
pz	0.517



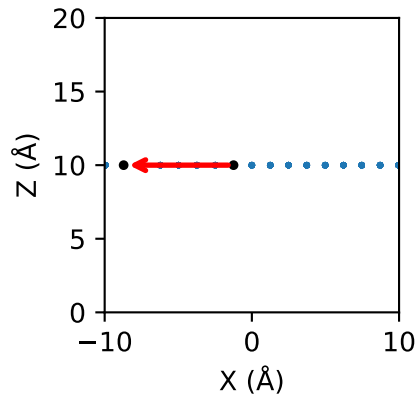
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, 4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	0.844

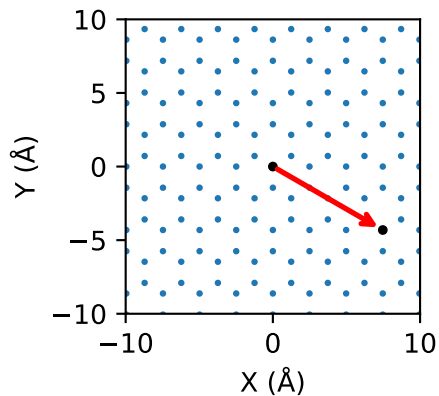


Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, 4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

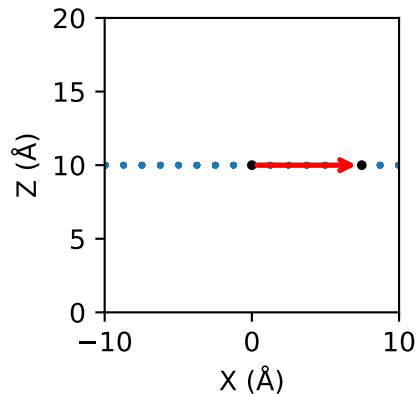


	pz
pz	0.844

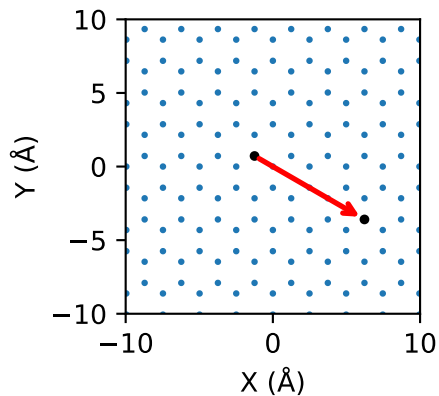




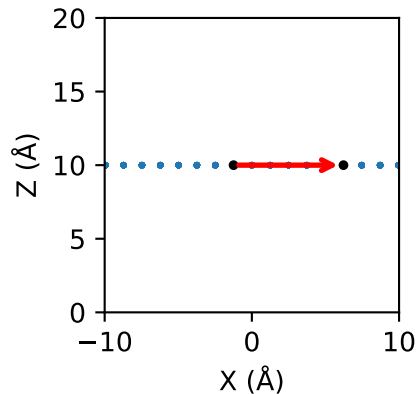
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (2, -2, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, -4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



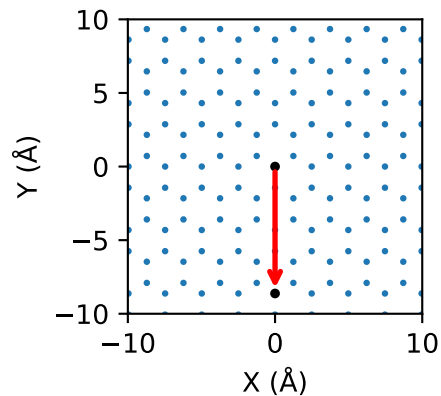
	pz
pz	0.844



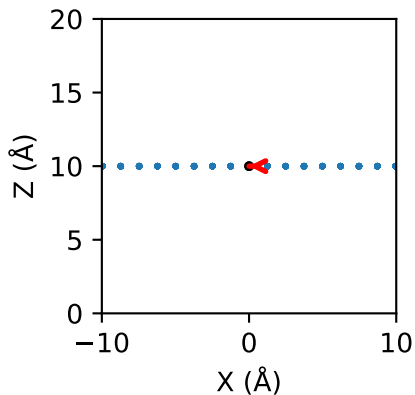
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (2, -2, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, -4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



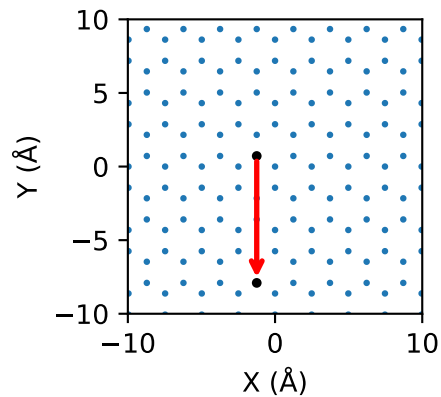
	pz
pz	0.844



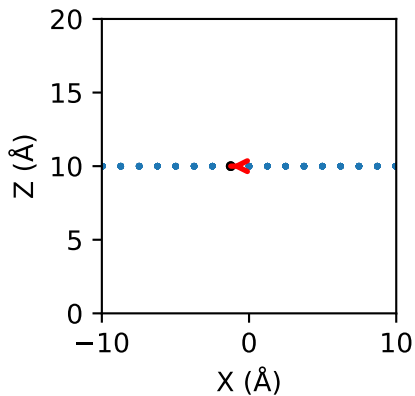
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-0.0, -8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



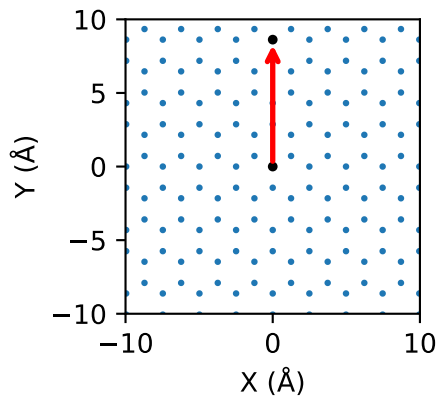
	pz
pz	0.843



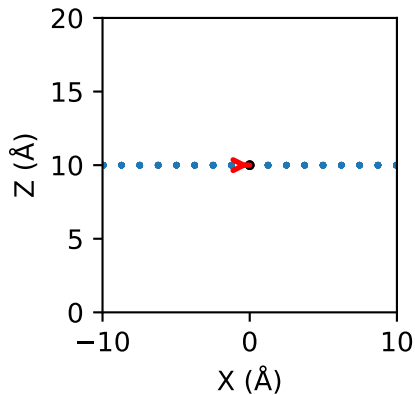
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (-2, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-0.0, -8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



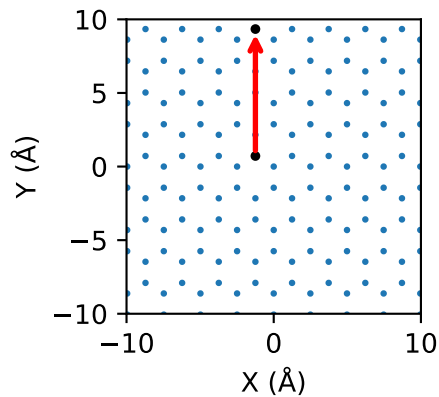
	pz
pz	0.843



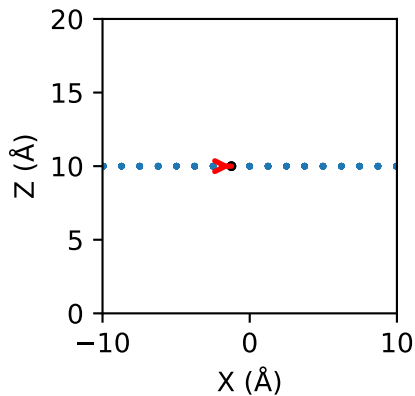
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (2, 4, 0)  
 Cartesian vector (rx, ry, rz) = (0.0, 8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



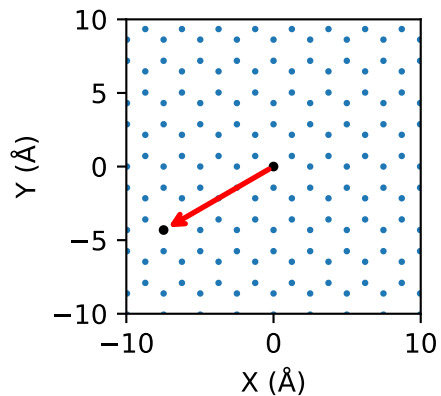
	pz
pz	0.843



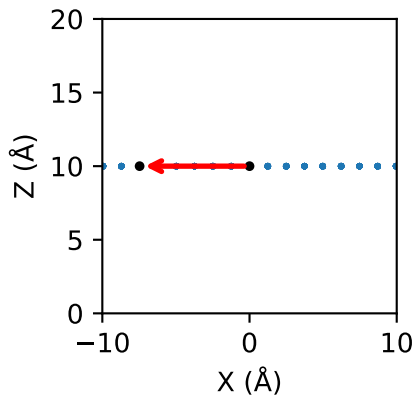
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (2, 4, 0)  
 Cartesian vector (rx, ry, rz) = (0.0, 8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



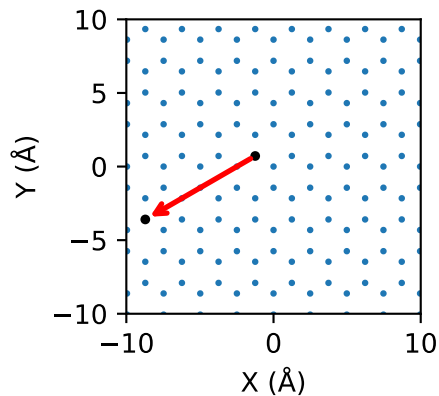
	pz
pz	0.843



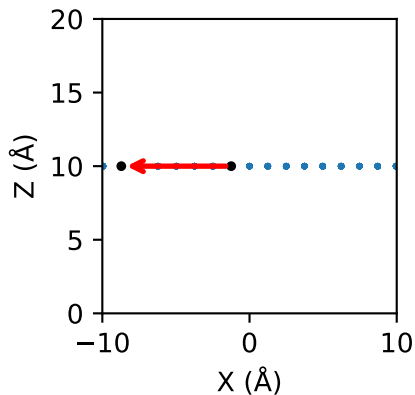
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, -4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	0.844

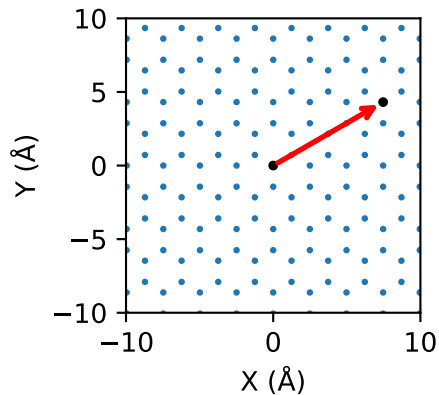


Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, -4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

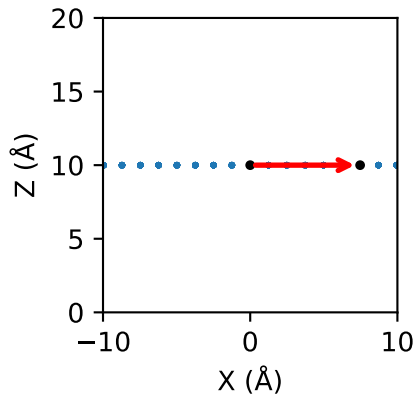


	pz
pz	0.844

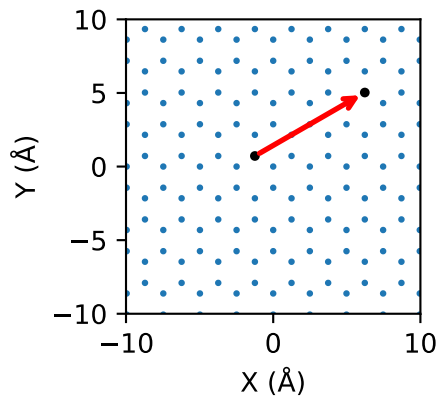




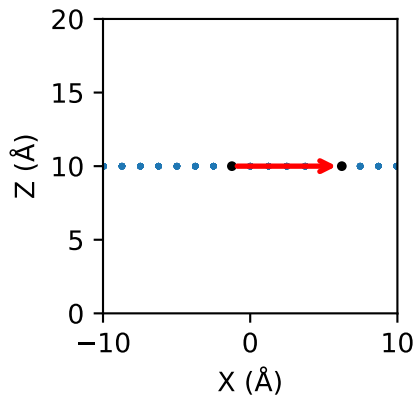
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (4, 2, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, 4.311, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



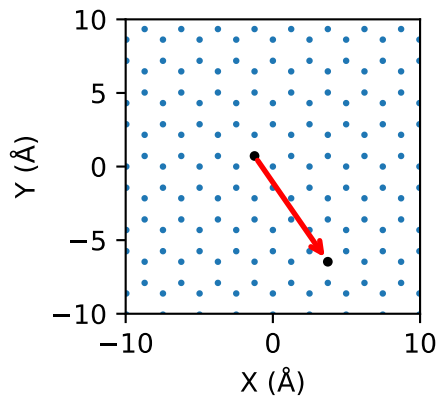
	pz
pz	0.844



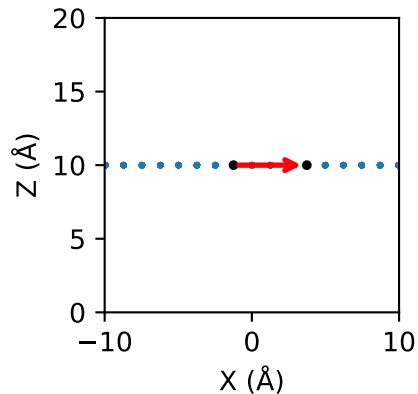
Distance = 8.622 Å  
 Cell vector (Rx, Ry, Rz) = (4, 2, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, 4.311, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



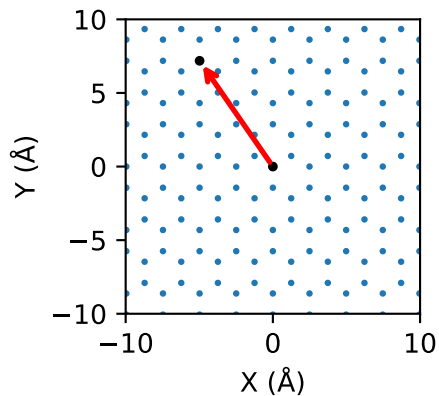
	pz
pz	0.844



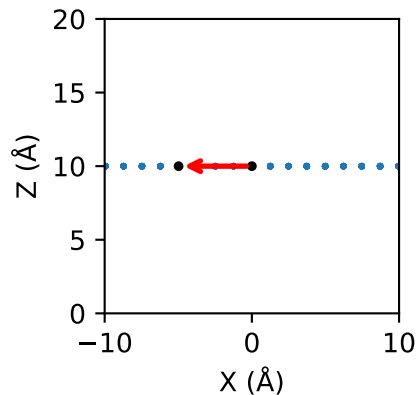
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (0, -3, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, -7.185, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



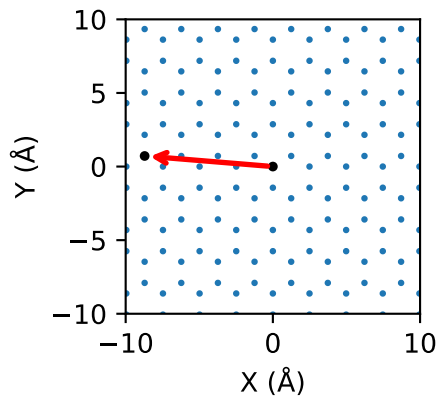
	pz
pz	6.171



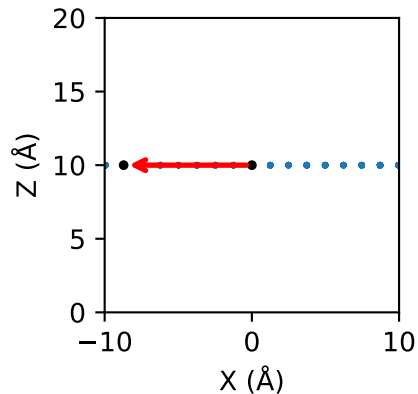
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (0, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 7.185, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



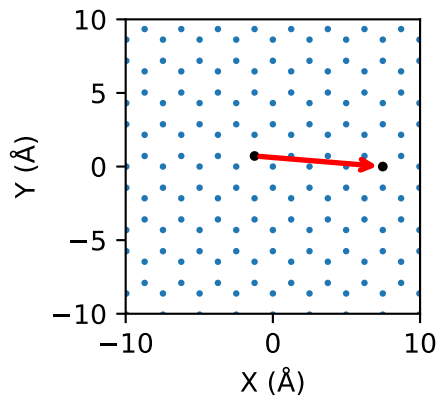
	pz
pz	6.171



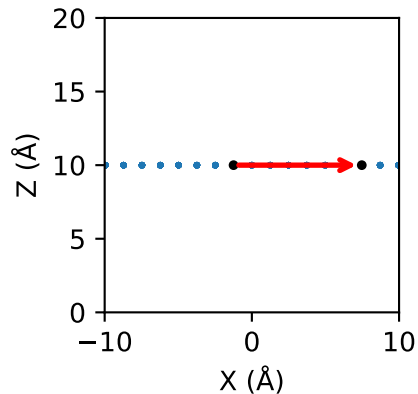
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (-3, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-8.711, 0.718, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



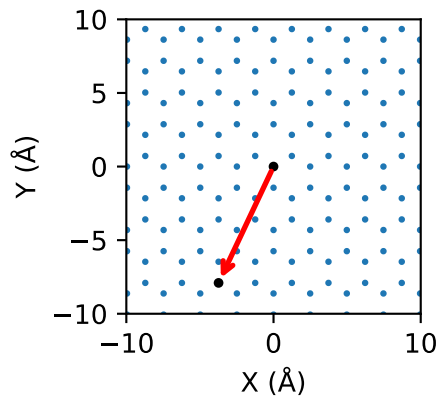
	pz
pz	6.172



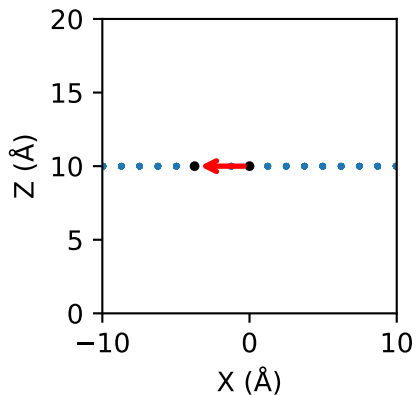
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (3, 0, 0)  
 Cartesian vector (rx, ry, rz) = (8.711, -0.718, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



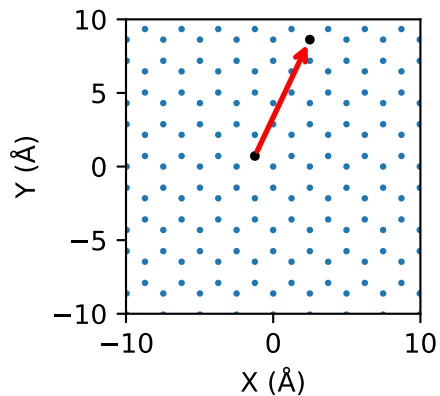
	pz
pz	6.172



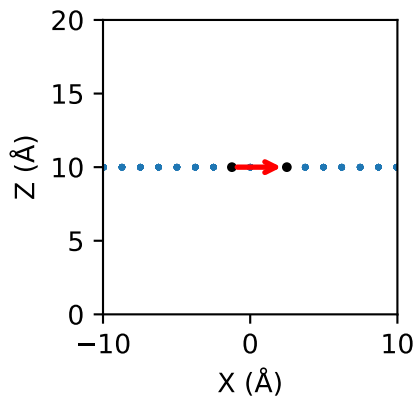
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-3.733, -7.904, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



	pz
pz	-0.338

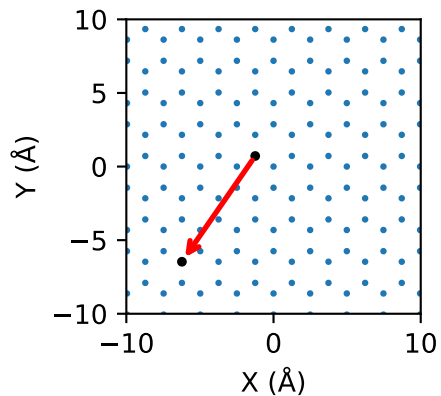


Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (3, 4, 0)  
 Cartesian vector (rx, ry, rz) = (3.733, 7.904, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV

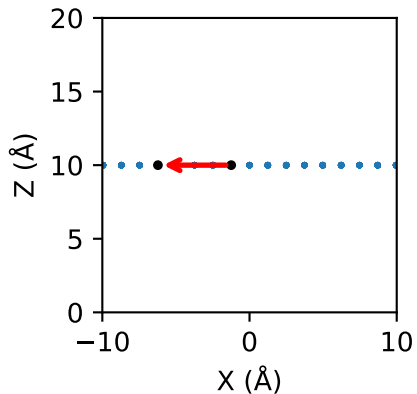


	pz
pz	-0.338

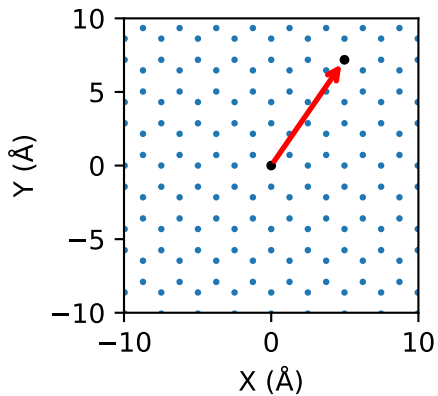




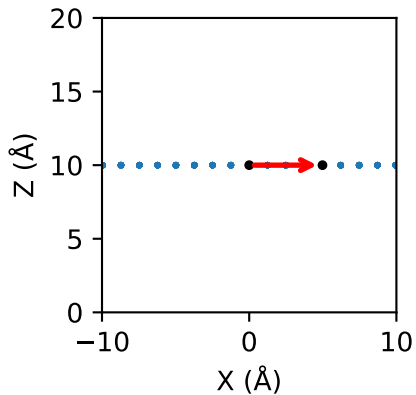
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, -7.185, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



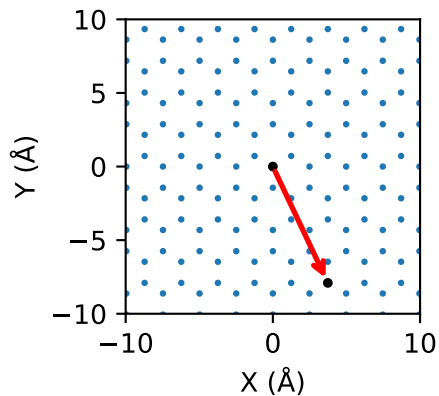
	pz
pz	-0.338



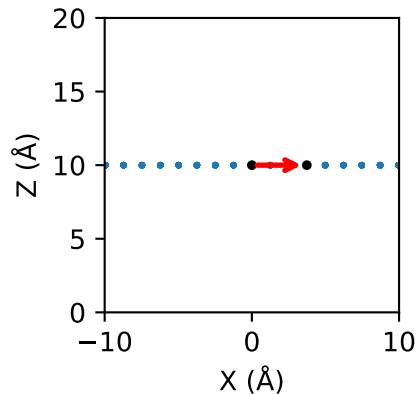
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (4, 3, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 7.185, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



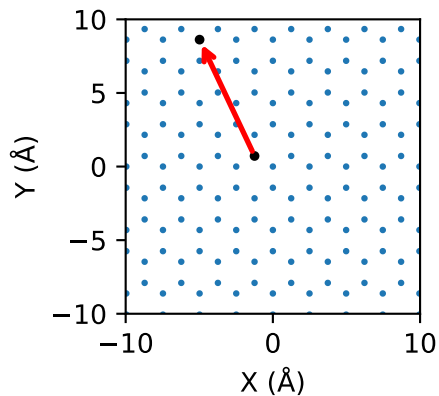
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pz	-0.338



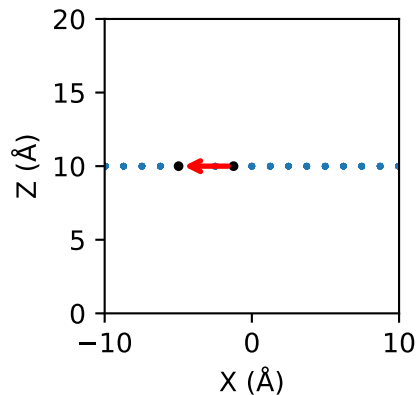
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (0, -4, 0)  
 Cartesian vector (rx, ry, rz) = (3.734, -7.904, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



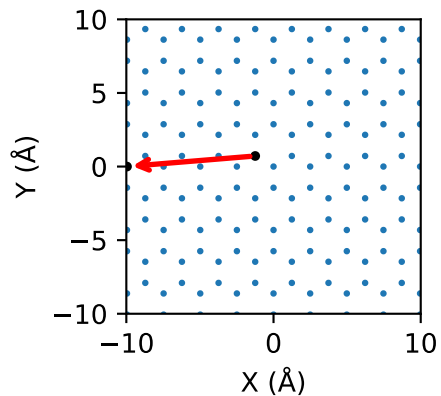
	pz
pz	-0.187



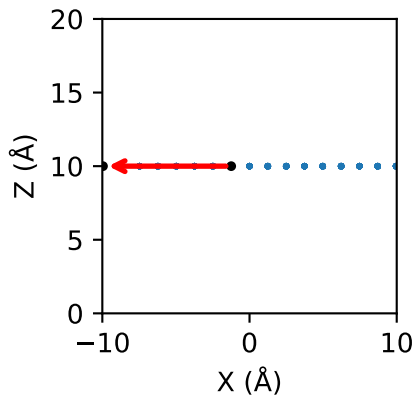
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (0, 4, 0)  
 Cartesian vector (rx, ry, rz) = (-3.734, 7.904, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



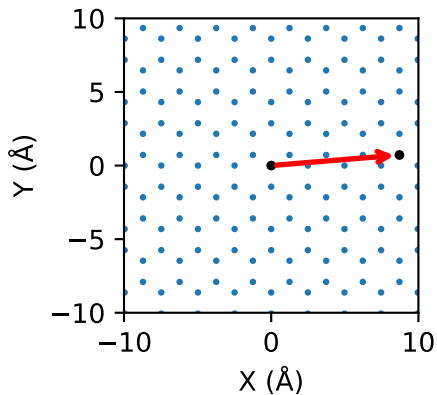
	pz
pz	-0.187



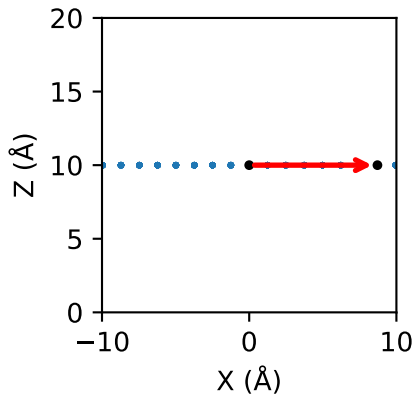
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (-4, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-8.712, -0.718, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



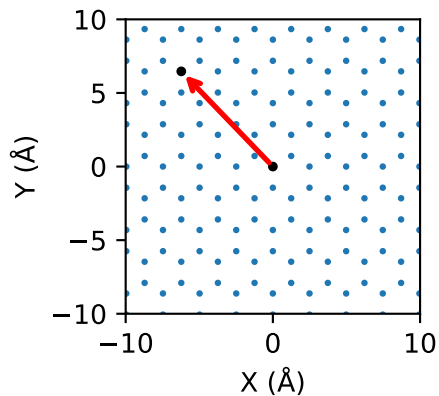
	pz
pz	-0.187



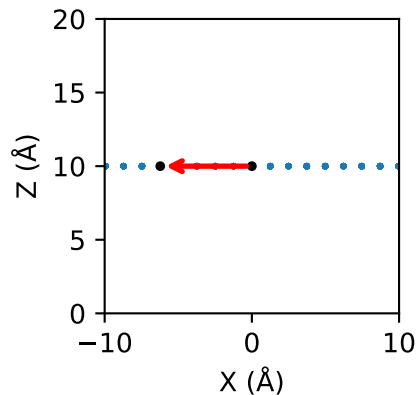
Distance = 8.741 Å  
 Cell vector (Rx, Ry, Rz) = (4, 0, 0)  
 Cartesian vector (rx, ry, rz) = (8.712, 0.718, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



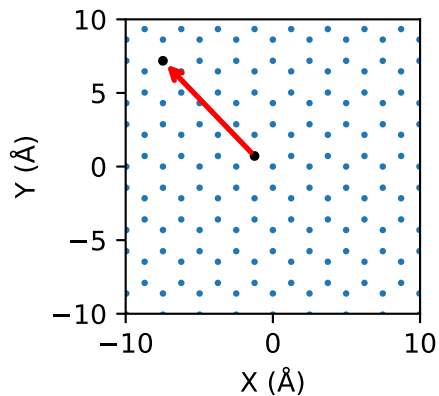
	pz
pz	-0.187



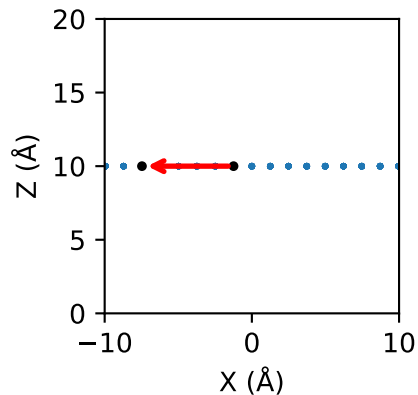
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, 6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-0.081

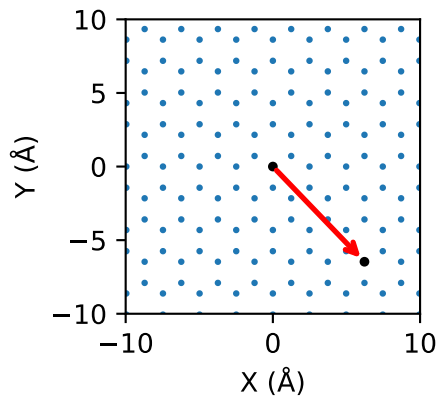


Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-1, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, 6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

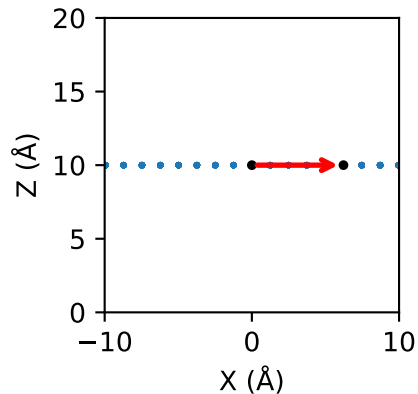


	pz
pz	-0.081

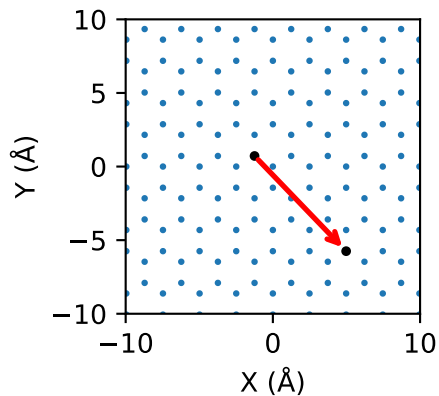




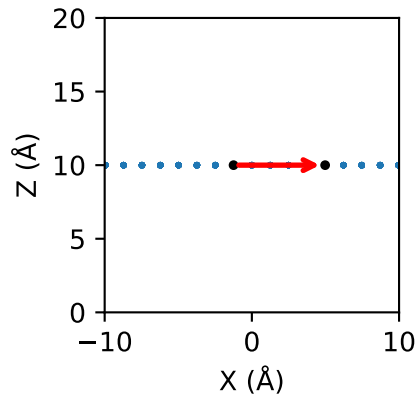
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (1, -3, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, -6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



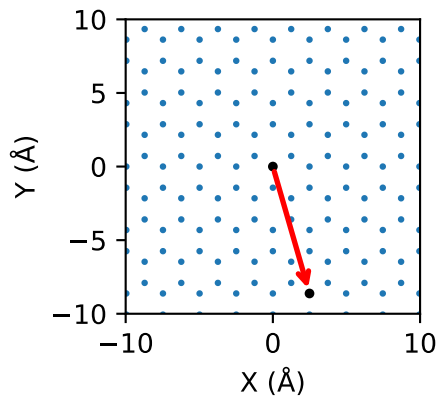
	pz
pz	-0.081



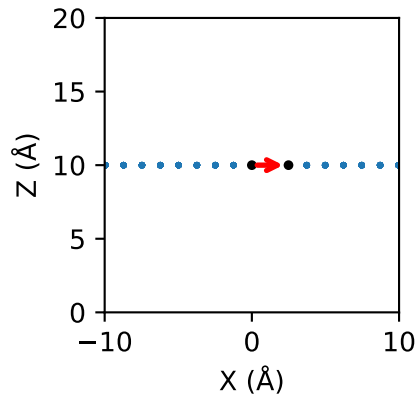
Distance = 8.974 Å  
 Cell vector ( $R_x$ ,  $R_y$ ,  $R_z$ ) = (1, -3, 0)  
 Cartesian vector ( $r_x$ ,  $r_y$ ,  $r_z$ ) = (6.223, -6.467, 0.0)  
 Atomic index ( $A_1$ ,  $A_2$ ) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



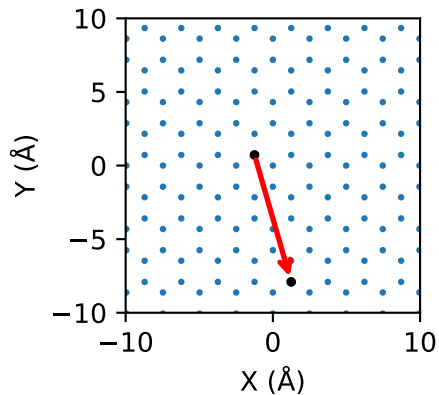
	pz
pz	-0.081



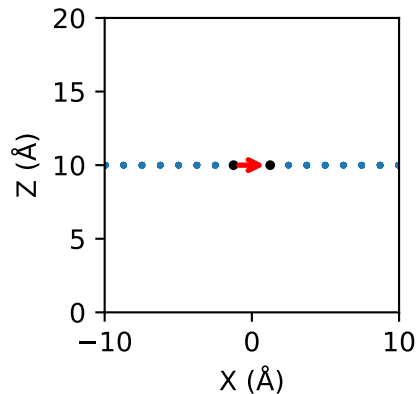
Distance = 8.974 Å  
 Cell vector ( $R_x$ ,  $R_y$ ,  $R_z$ ) = (-1, -4, 0)  
 Cartesian vector ( $r_x$ ,  $r_y$ ,  $r_z$ ) = (2.489, -8.622, 0.0)  
 Atomic index ( $A_1$ ,  $A_2$ ) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



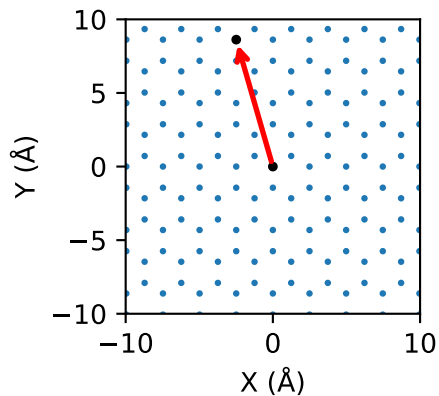
	pz
pz	-0.081



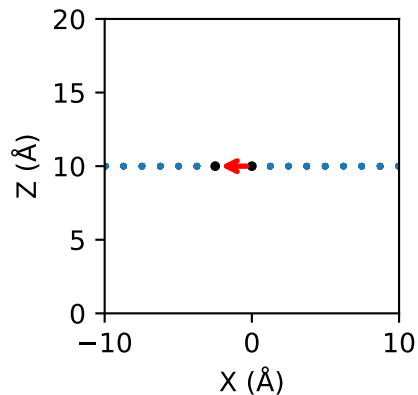
Distance = 8.974 Å  
 Cell vector ( $R_x$ ,  $R_y$ ,  $R_z$ ) = (-1, -4, 0)  
 Cartesian vector ( $r_x$ ,  $r_y$ ,  $r_z$ ) = (2.489, -8.622, 0.0)  
 Atomic index ( $A_1$ ,  $A_2$ ) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



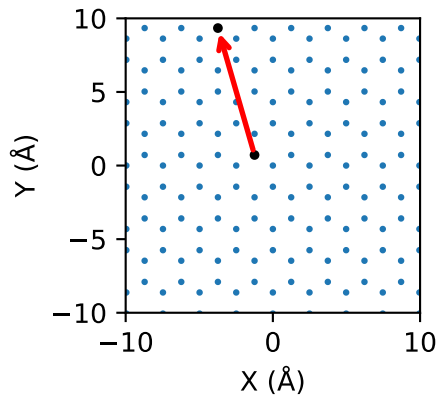
	pz
pz	-0.081



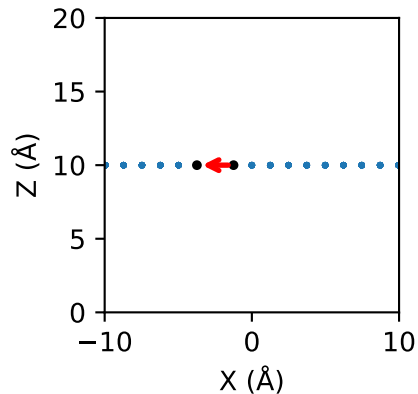
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (1, 4, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



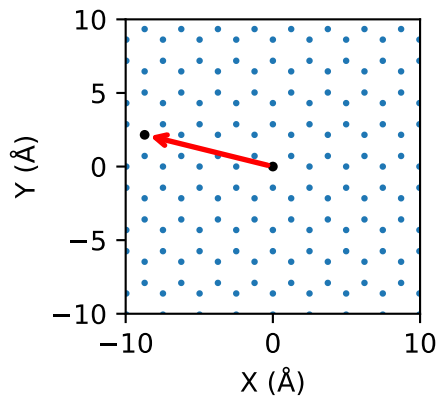
	pz
pz	-0.081



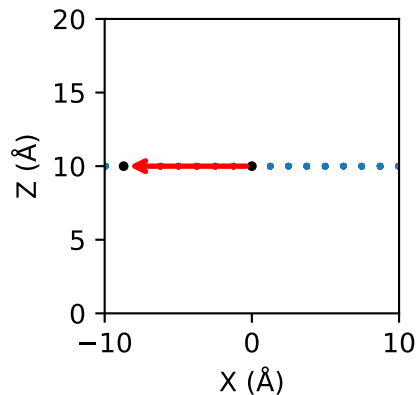
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (1, 4, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, 8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



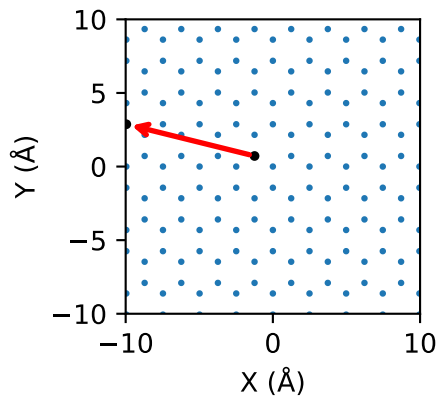
	pz
pz	-0.081



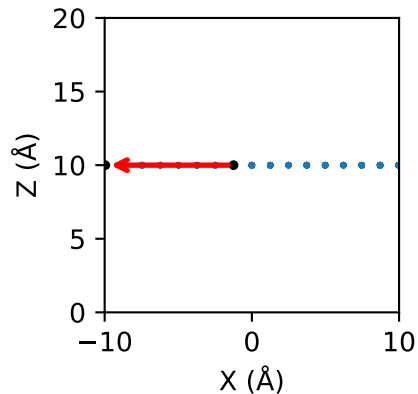
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-3, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-8.712, 2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-0.081

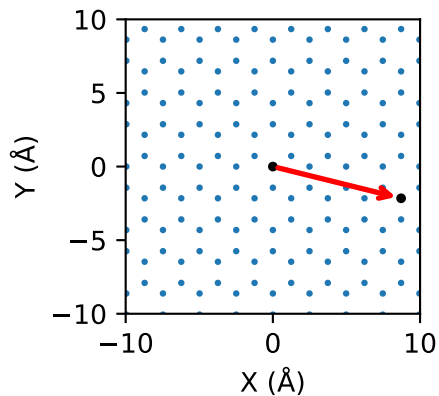


Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-3, 1, 0)  
 Cartesian vector (rx, ry, rz) = (-8.712, 2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

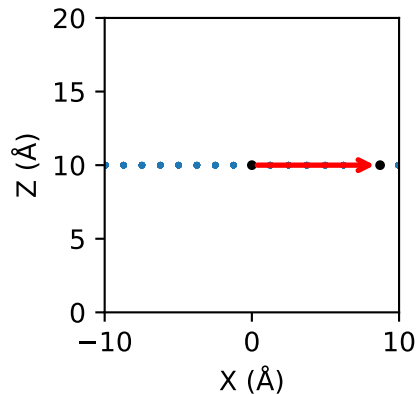


	pz
pz	-0.081

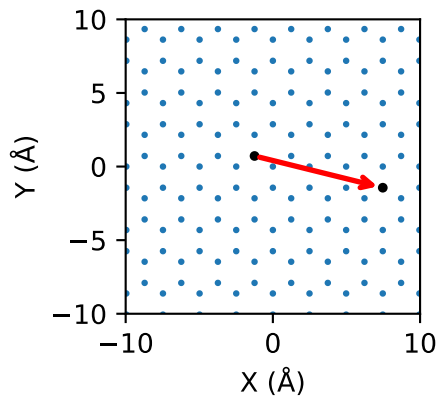




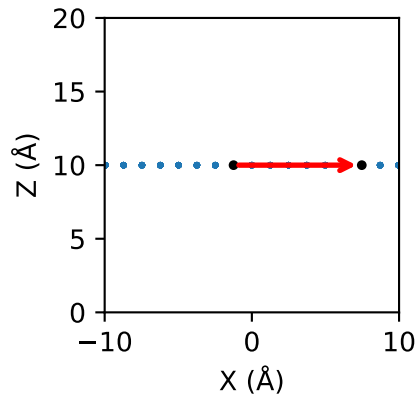
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (3, -1, 0)  
 Cartesian vector (rx, ry, rz) = (8.712, -2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



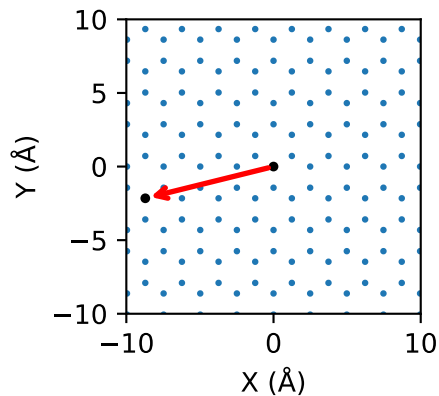
	pz
pz	-0.081



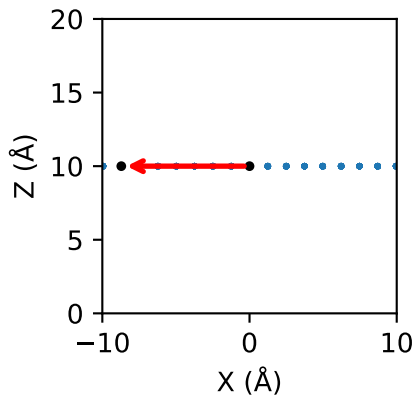
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (3, -1, 0)  
 Cartesian vector (rx, ry, rz) = (8.712, -2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



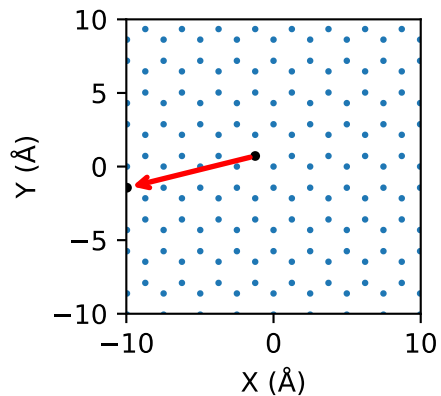
	pz
pz	-0.081



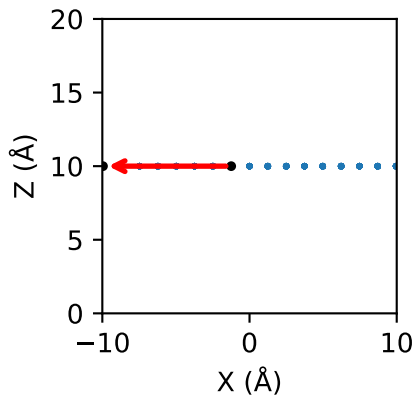
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-8.712, -2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



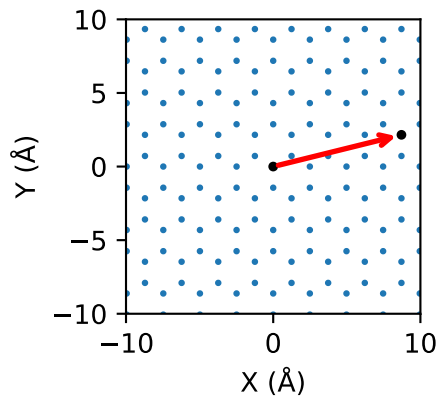
	pz
pz	-0.081



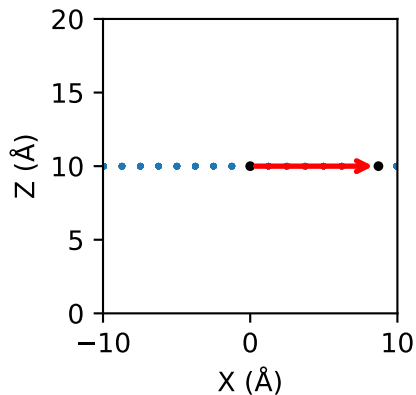
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -1, 0)  
 Cartesian vector (rx, ry, rz) = (-8.712, -2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



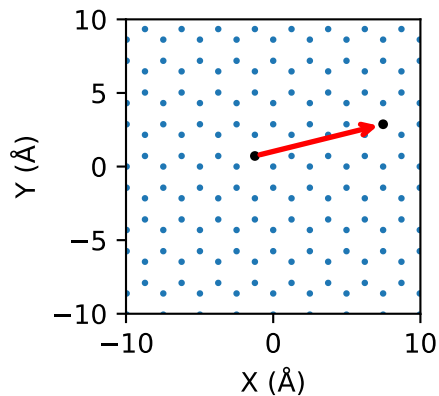
	pz
pz	-0.081



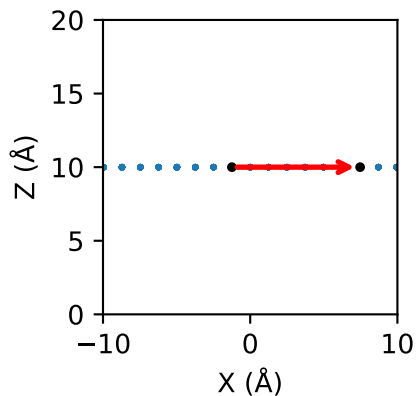
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (4, 1, 0)  
 Cartesian vector (rx, ry, rz) = (8.712, 2.156, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



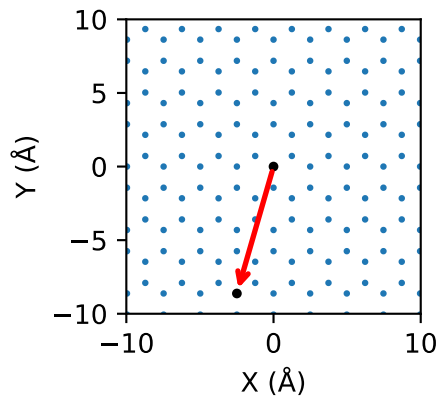
	pz
pz	-0.081



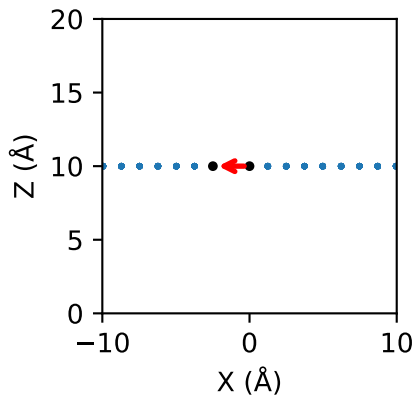
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (4, 1, 0)  
 Cartesian vector (rx, ry, rz) = (8.712, 2.156, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



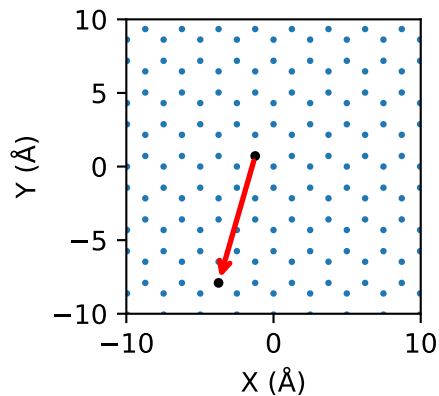
	pz
pz	-0.081



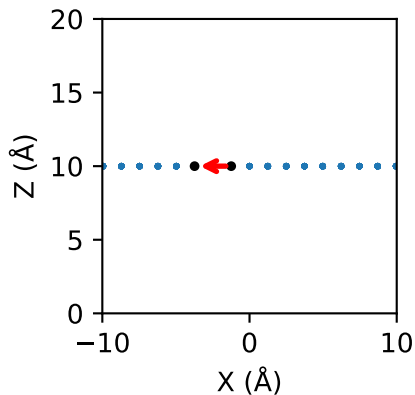
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, -8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-0.081

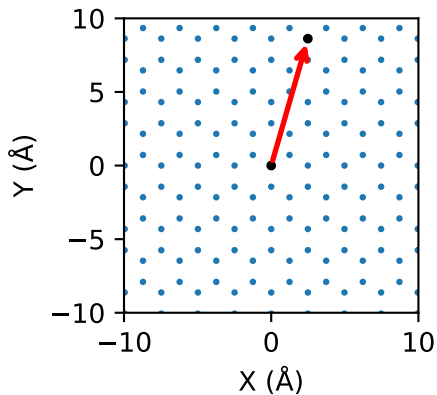


Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-2.489, -8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

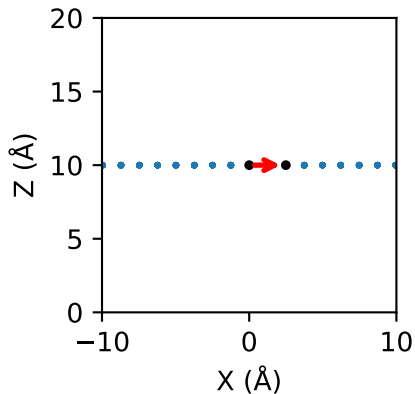


	pz
pz	-0.081

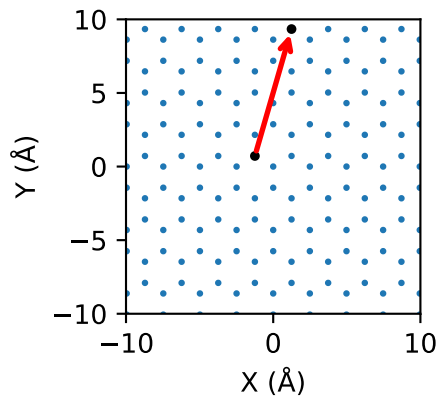




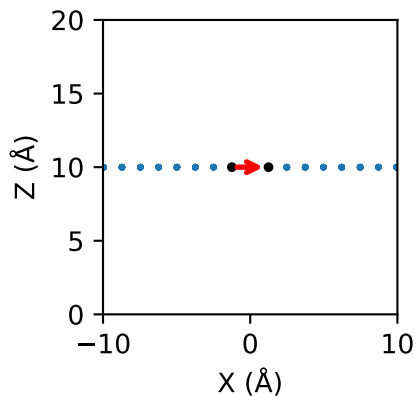
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (3, 4, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



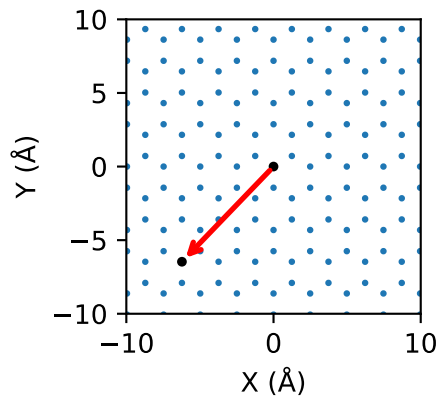
	pz
pz	-0.081



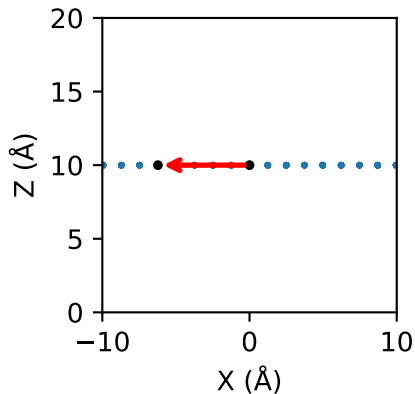
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (3, 4, 0)  
 Cartesian vector (rx, ry, rz) = (2.489, 8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



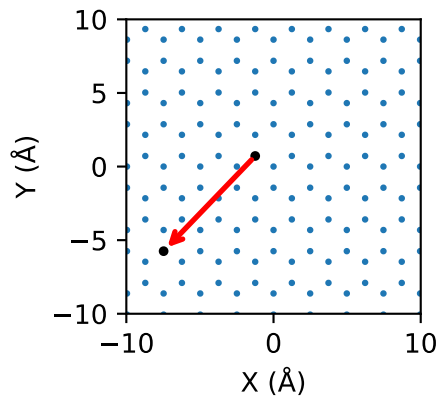
	pz
pz	-0.081



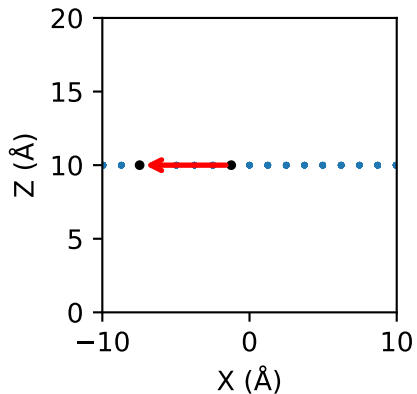
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, -6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



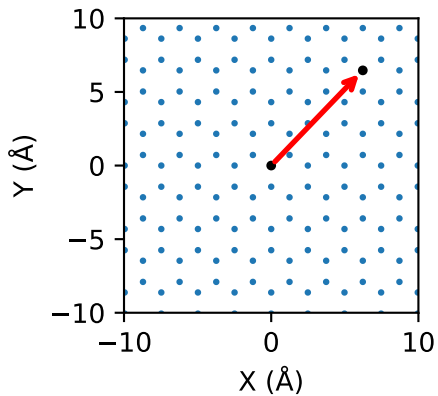
	pz
pz	-0.082



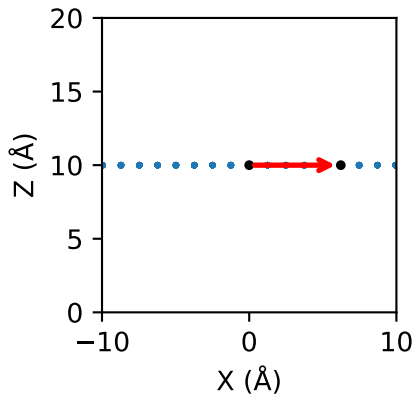
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-6.223, -6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



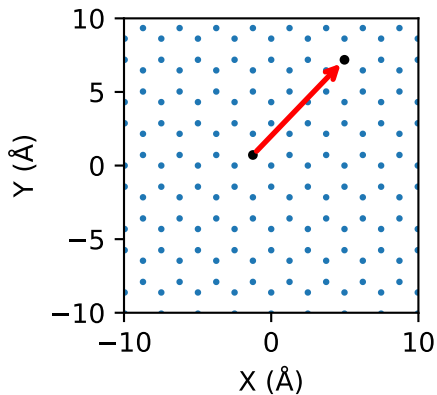
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pz	-0.082



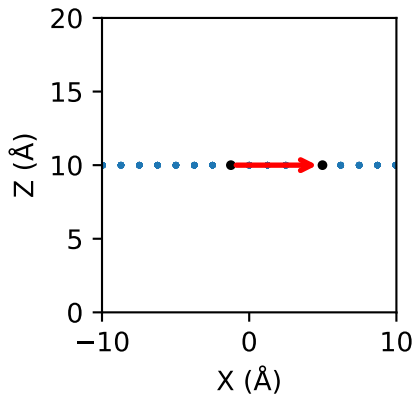
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (4, 3, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, 6.467, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



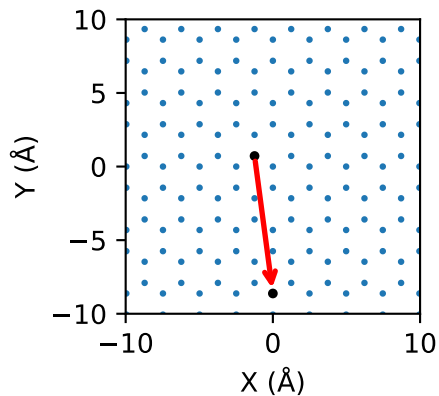
	pz
pz	-0.082



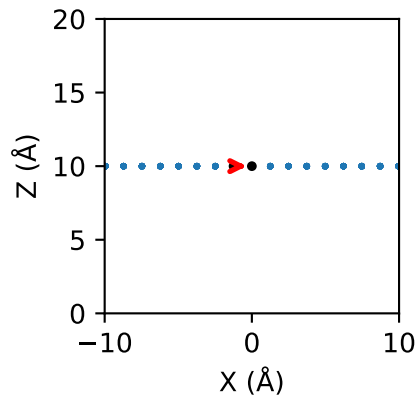
Distance = 8.974 Å  
 Cell vector (Rx, Ry, Rz) = (4, 3, 0)  
 Cartesian vector (rx, ry, rz) = (6.223, 6.467, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



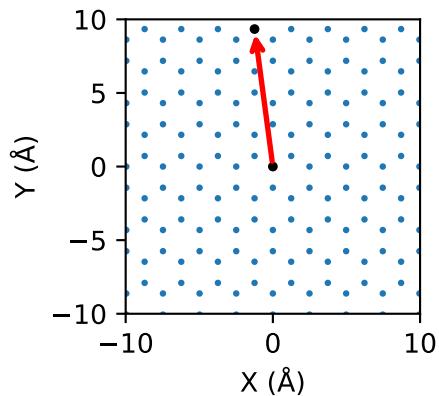
	pz
pz	-0.082



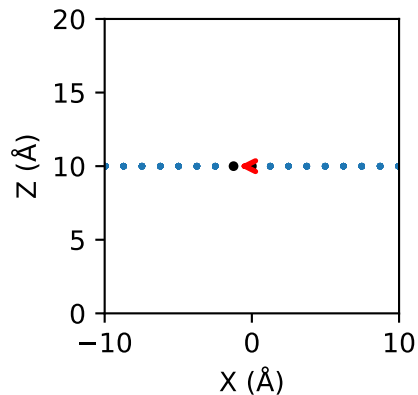
Distance = 9.423 Å  
 Cell vector ( $R_x$ ,  $R_y$ ,  $R_z$ ) = (-2, -4, 0)  
 Cartesian vector ( $r_x$ ,  $r_y$ ,  $r_z$ ) = (1.244, -9.341, 0.0)  
 Atomic index ( $A_1$ ,  $A_2$ ) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-1.479

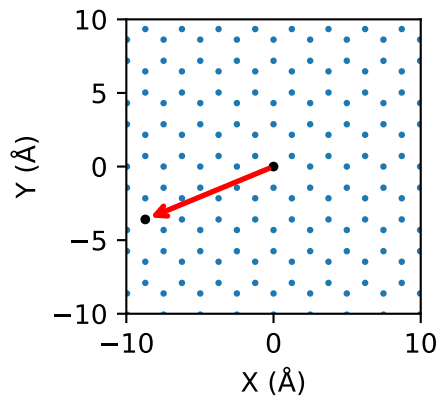


Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (2, 4, 0)  
 Cartesian vector (rx, ry, rz) = (-1.244, 9.341, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

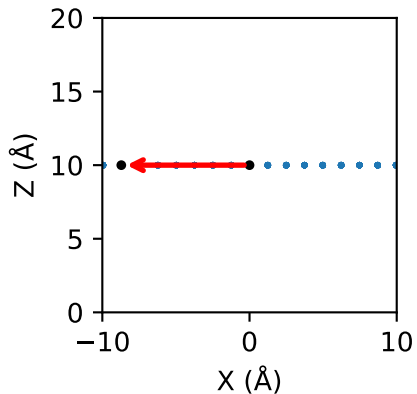


	pz
pz	-1.479

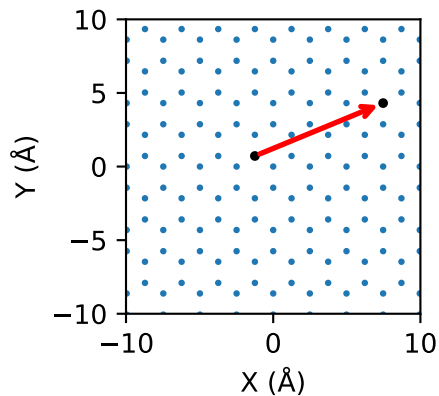




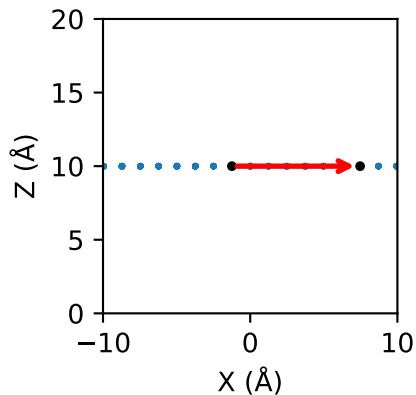
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -2, 0)  
 Cartesian vector (rx, ry, rz) = (-8.711, -3.593, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



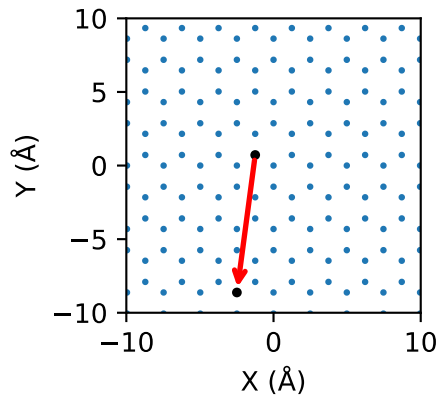
	pz
pz	-1.48



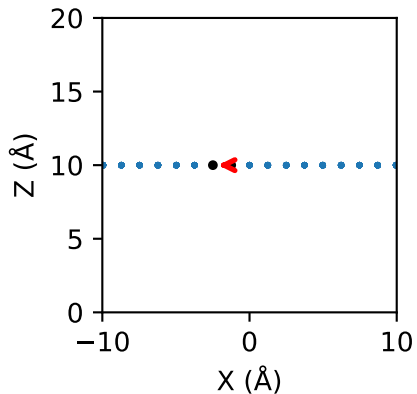
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (4, 2, 0)  
 Cartesian vector (rx, ry, rz) = (8.711, 3.593, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



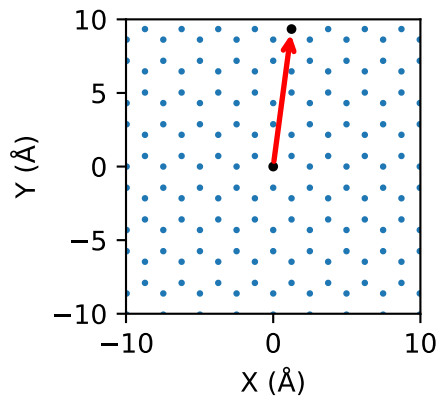
	pz
pz	-1.48



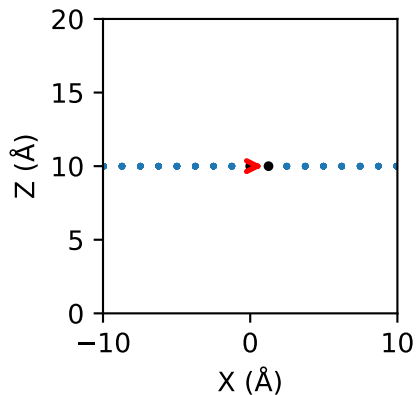
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (-3, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-1.245, -9.341, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



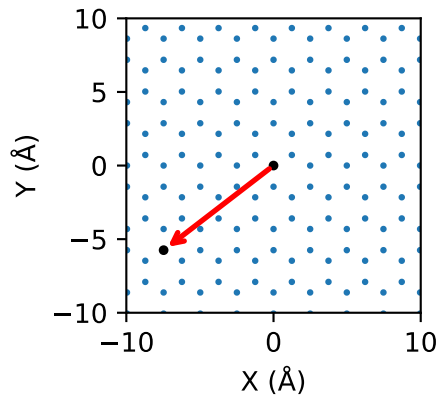
	pz
pz	0.326



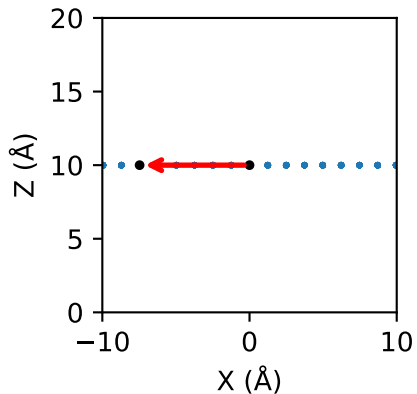
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (3, 4, 0)  
 Cartesian vector (rx, ry, rz) = (1.245, 9.341, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



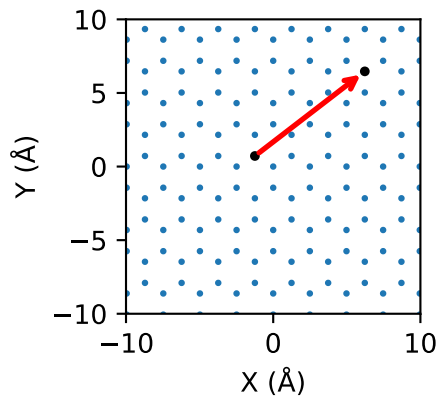
	pz
pz	0.326



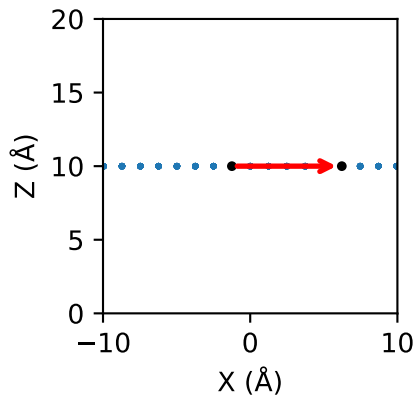
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -3, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, -5.748, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



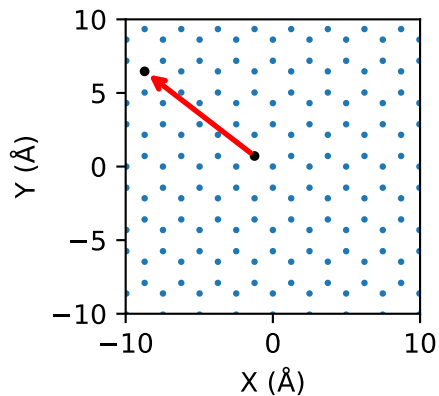
	pz
pz	0.326



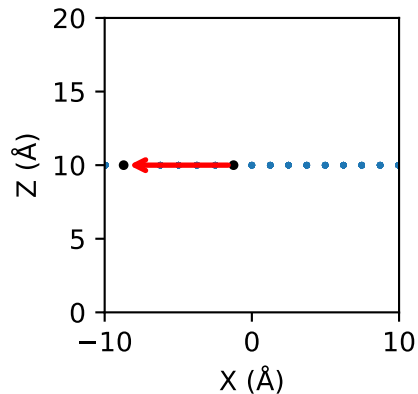
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (4, 3, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, 5.748, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



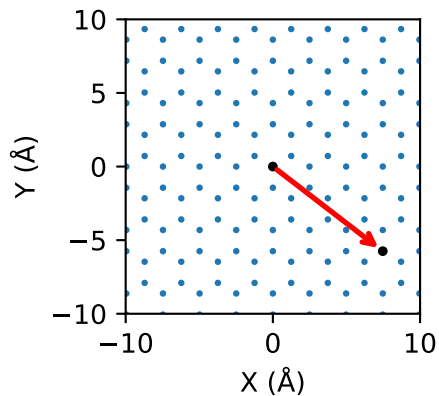
	pz
pz	0.326



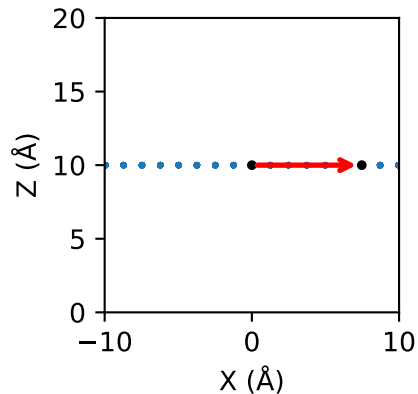
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (-2, 3, 0)  
 Cartesian vector (rx, ry, rz) = (-7.467, 5.748, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	0.087

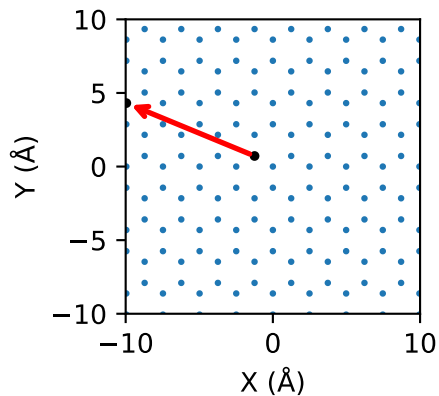


Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (2, -3, 0)  
 Cartesian vector (rx, ry, rz) = (7.467, -5.748, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV

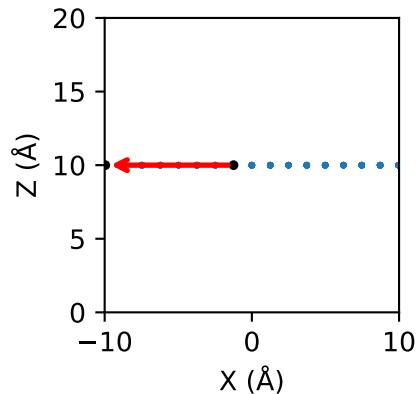


	pz
pz	0.087

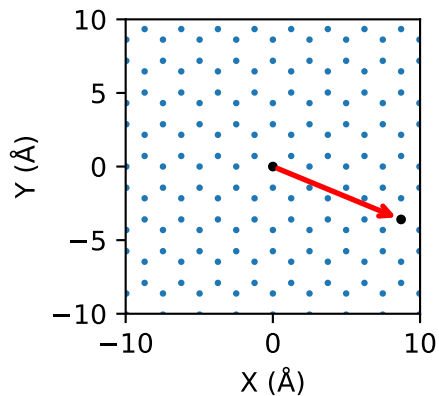




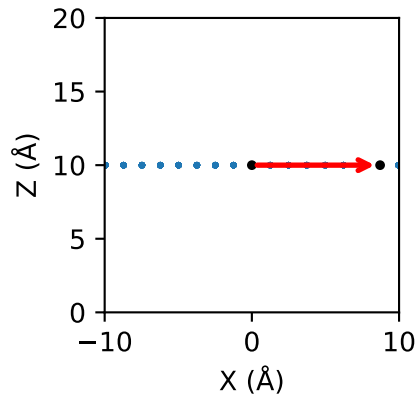
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (-3, 2, 0)  
 Cartesian vector (rx, ry, rz) = (-8.712, 3.593, 0.0)  
 Atomic index (A1, A2) = (1, 2)  
 from atom 2 to atom 1  
 Hamiltonian Unit: meV



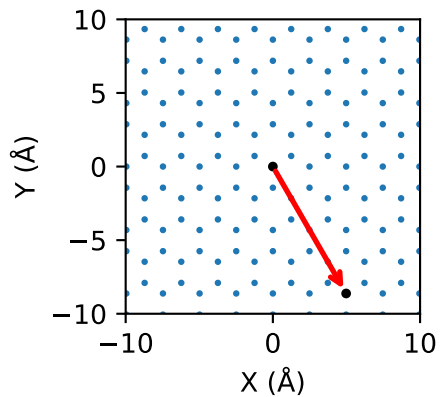
	pz
pz	0.087



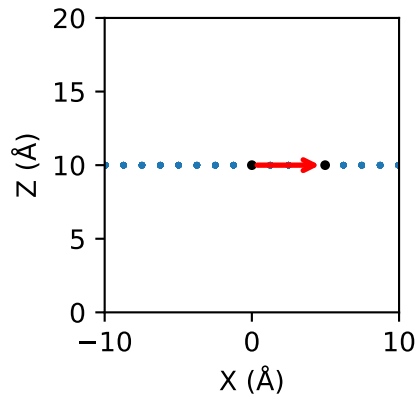
Distance = 9.423 Å  
 Cell vector (Rx, Ry, Rz) = (3, -2, 0)  
 Cartesian vector (rx, ry, rz) = (8.712, -3.593, 0.0)  
 Atomic index (A1, A2) = (2, 1)  
 from atom 1 to atom 2  
 Hamiltonian Unit: meV



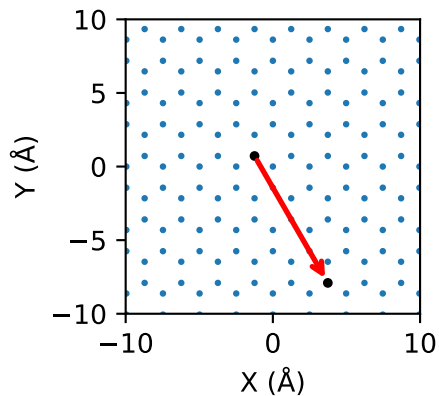
	pz
pz	0.087



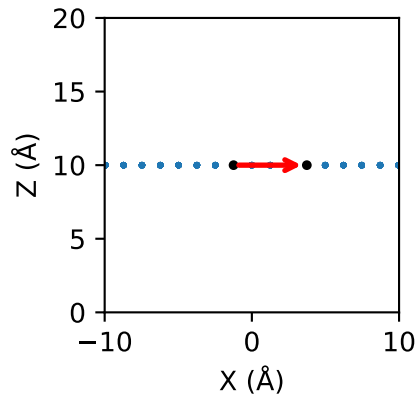
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (0, -4, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, -8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



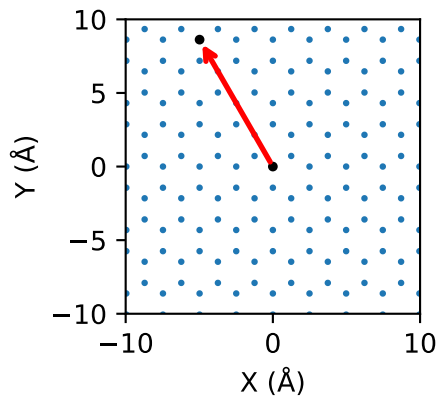
	pz
pz	-0.136



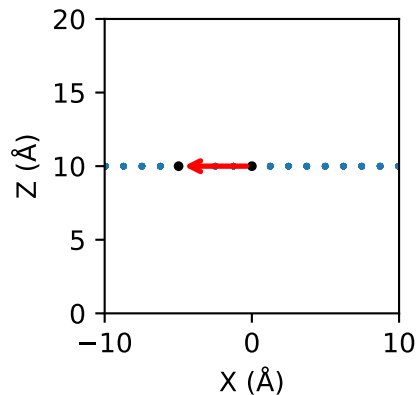
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (0, -4, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, -8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



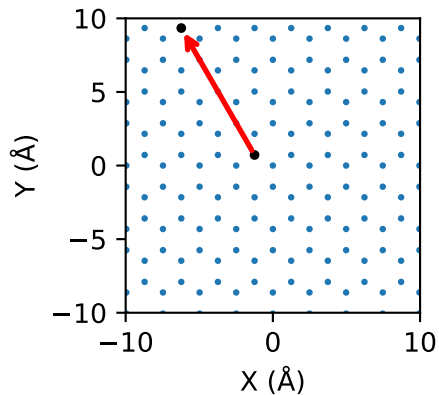
	pz
pz	-0.136



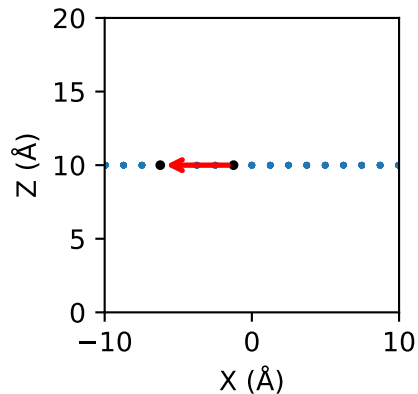
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (0, 4, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



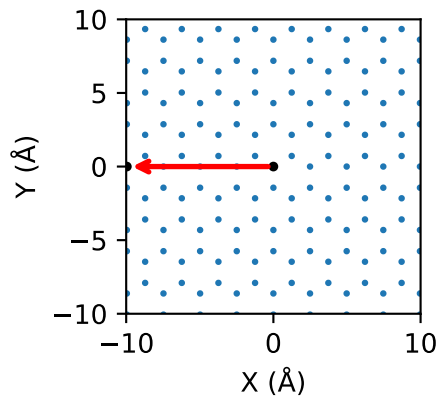
	pz
pz	-0.136



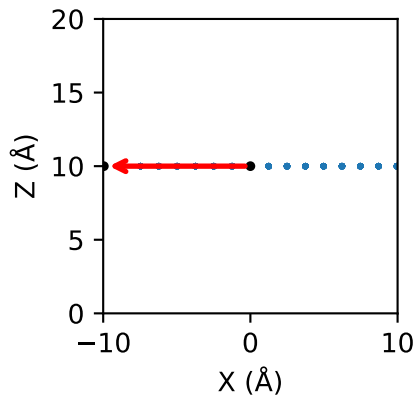
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (0, 4, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, 8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



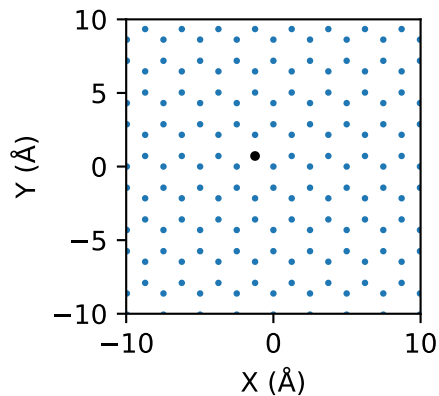
	pz
pz	-0.136



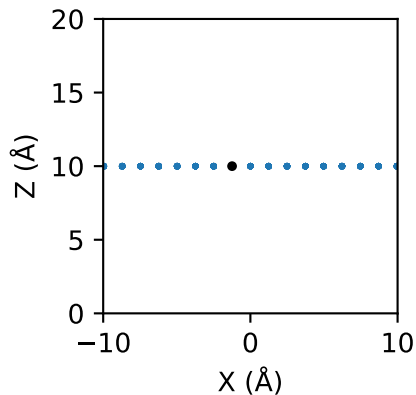
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (-4, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-9.956, 0.0, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-0.136

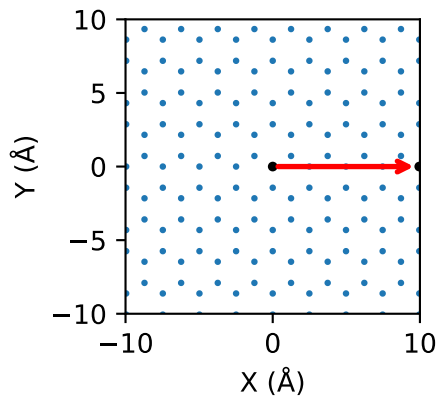


Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (-4, 0, 0)  
 Cartesian vector (rx, ry, rz) = (-9.956, 0.0, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV

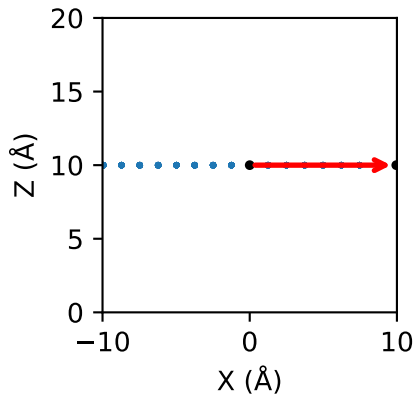


	pz
pz	-0.136

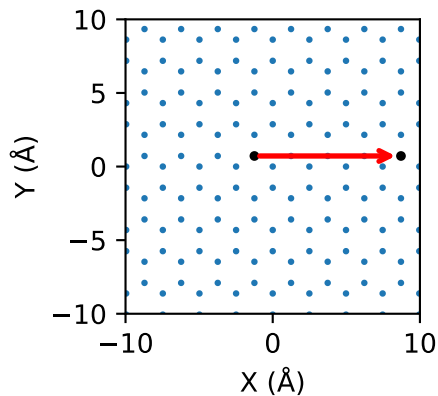




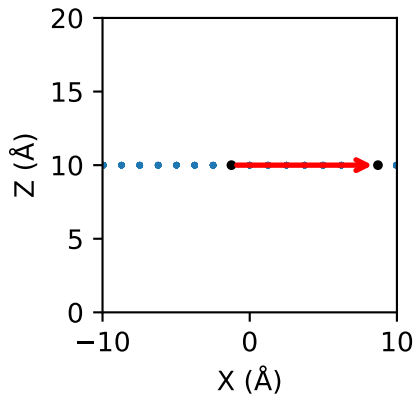
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (4, 0, 0)  
 Cartesian vector (rx, ry, rz) = (9.956, 0.0, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



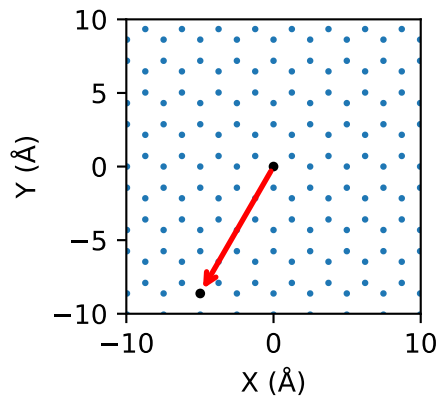
	pz
pz	-0.136



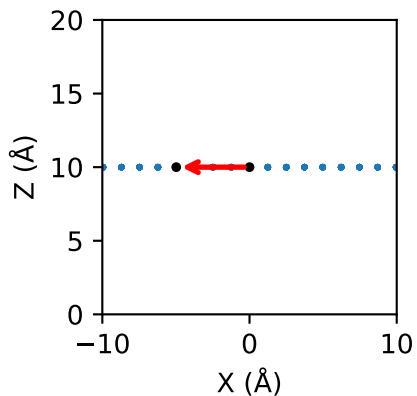
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (4, 0, 0)  
 Cartesian vector (rx, ry, rz) = (9.956, 0.0, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



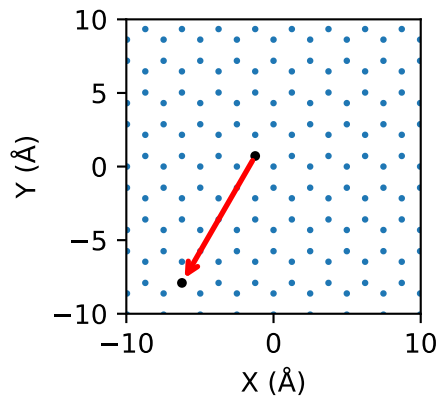
	pz
pz	-0.136



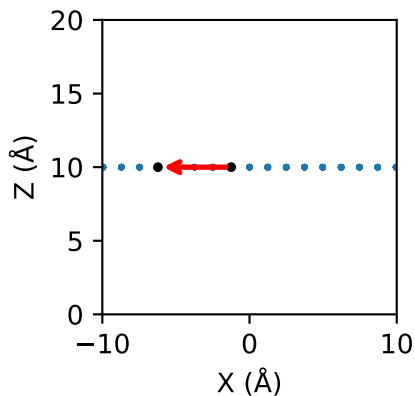
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, -8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



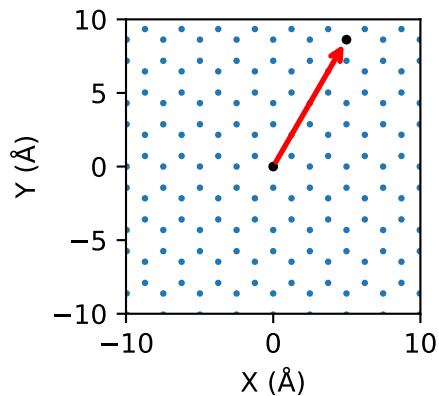
	pz
pz	-0.135



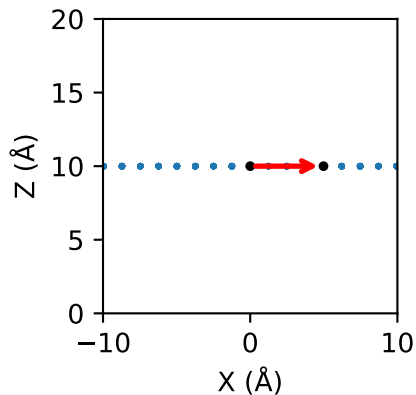
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (-4, -4, 0)  
 Cartesian vector (rx, ry, rz) = (-4.978, -8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



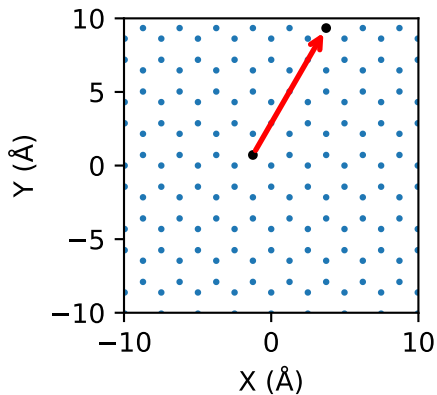
	pz
pz	-0.135



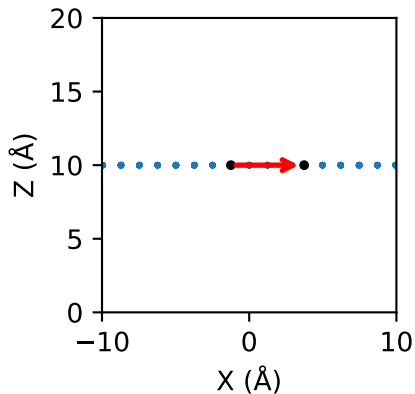
Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (4, 4, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 8.622, 0.0)  
 Atomic index (A1, A2) = (1, 1)  
 from atom 1 to atom 1  
 Hamiltonian Unit: meV



	pz
pz	-0.135



Distance = 9.956 Å  
 Cell vector (Rx, Ry, Rz) = (4, 4, 0)  
 Cartesian vector (rx, ry, rz) = (4.978, 8.622, 0.0)  
 Atomic index (A1, A2) = (2, 2)  
 from atom 2 to atom 2  
 Hamiltonian Unit: meV



	pz
pz	-0.135