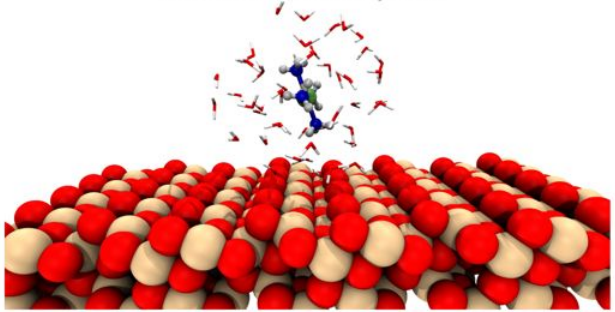
Introduction to electronic structure calculations

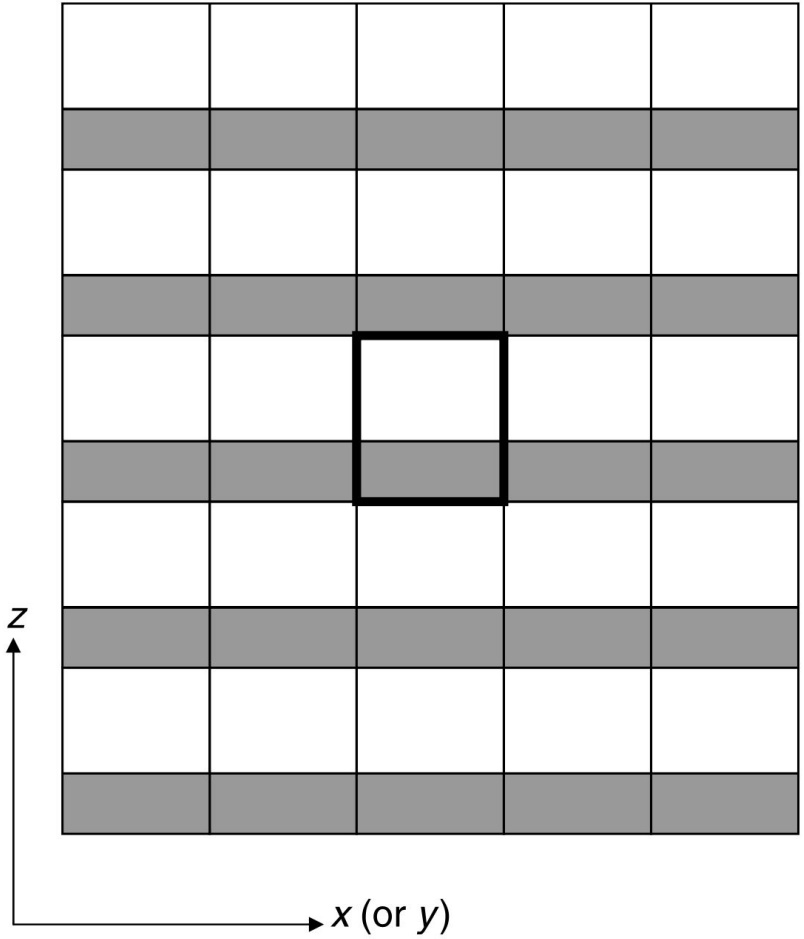
QM/MM and ab initio Molecular Dynamics
Summer School
June 23 – June 27, 2025

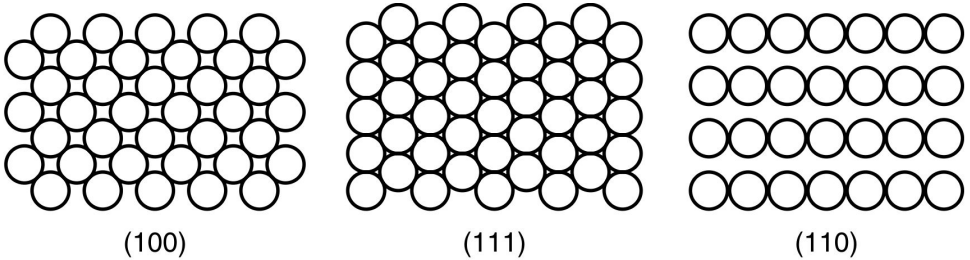


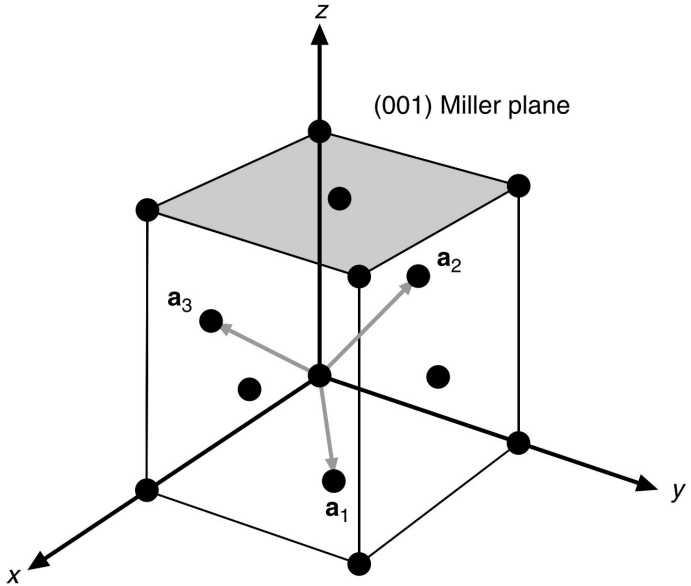
Creating surfaces and defects

Mario F. Borunda

Surfaces:

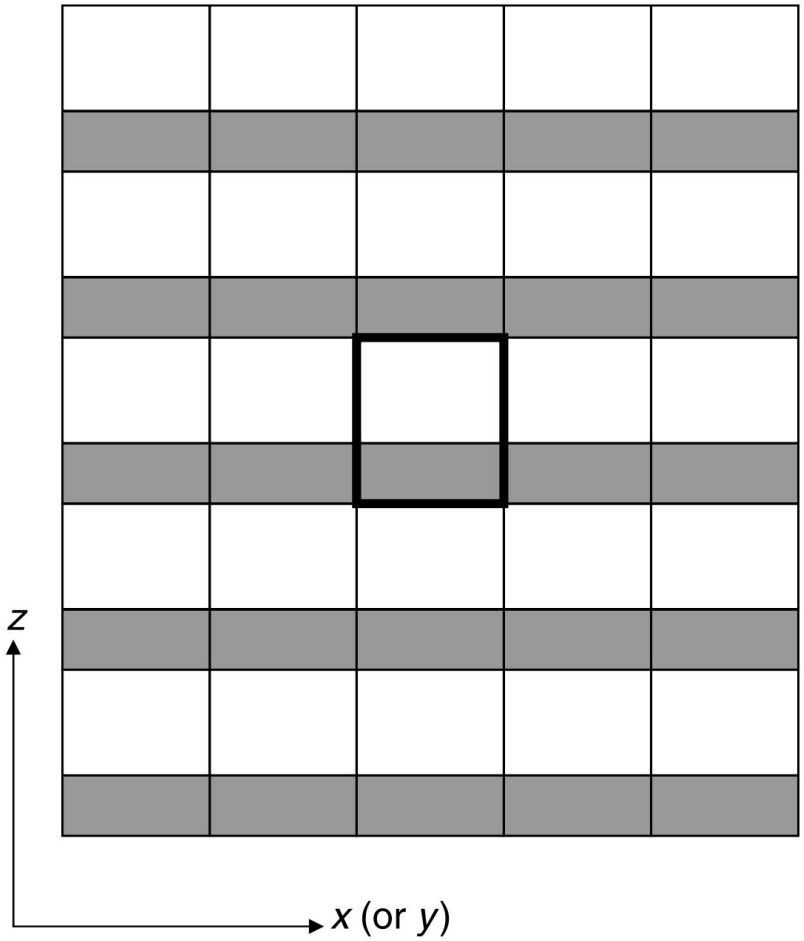


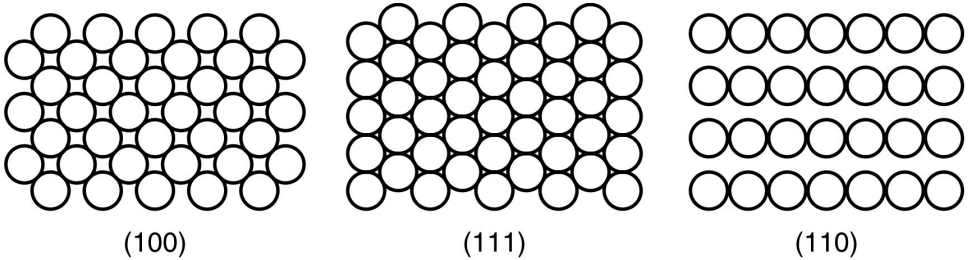


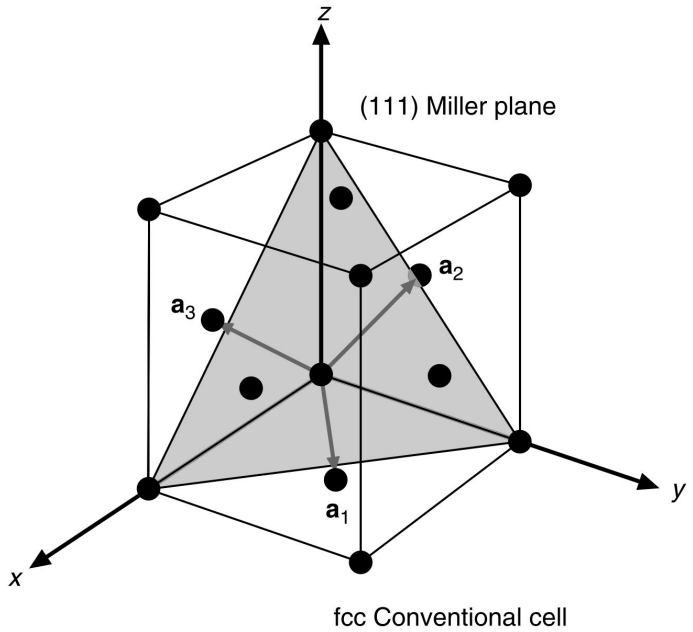


fcc Conventional cell

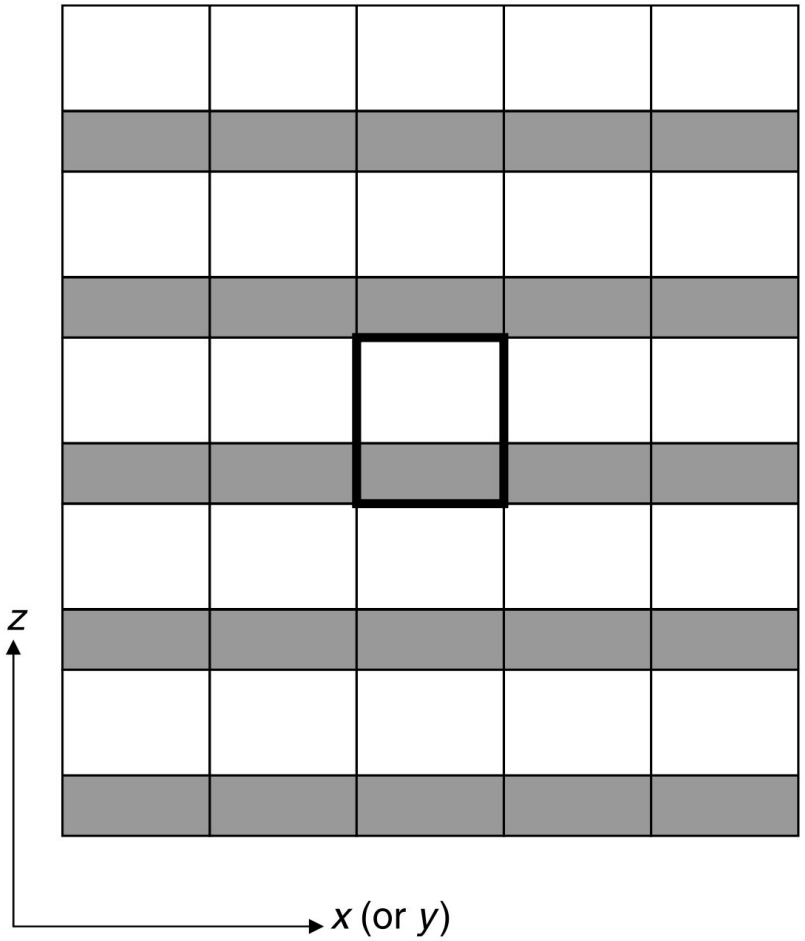
Surfaces:

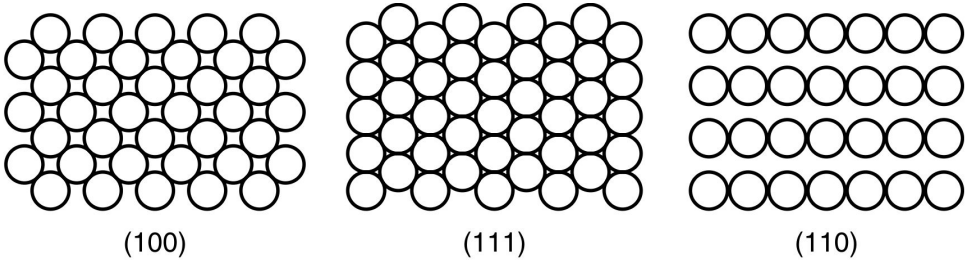

z
x (or y)

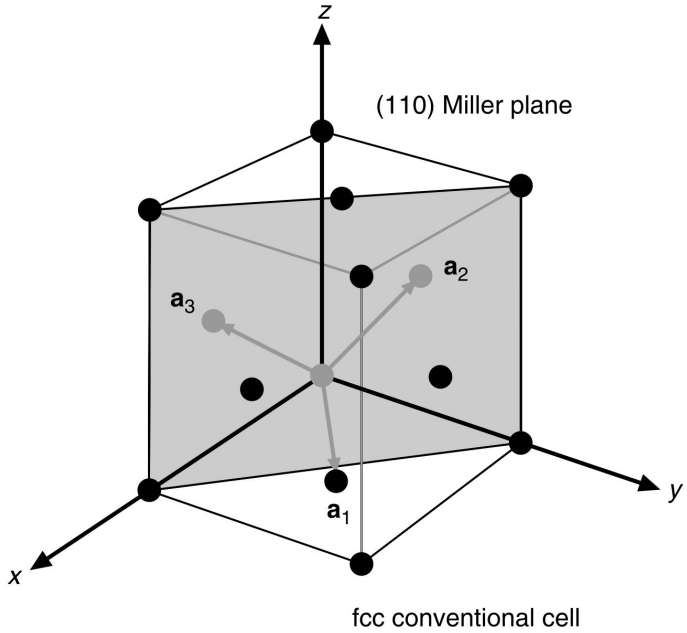

(100)
(111)
(110)


z
(111) Miller plane
a2
a3
a1
x
y
fcc Conventional cell

Surfaces:



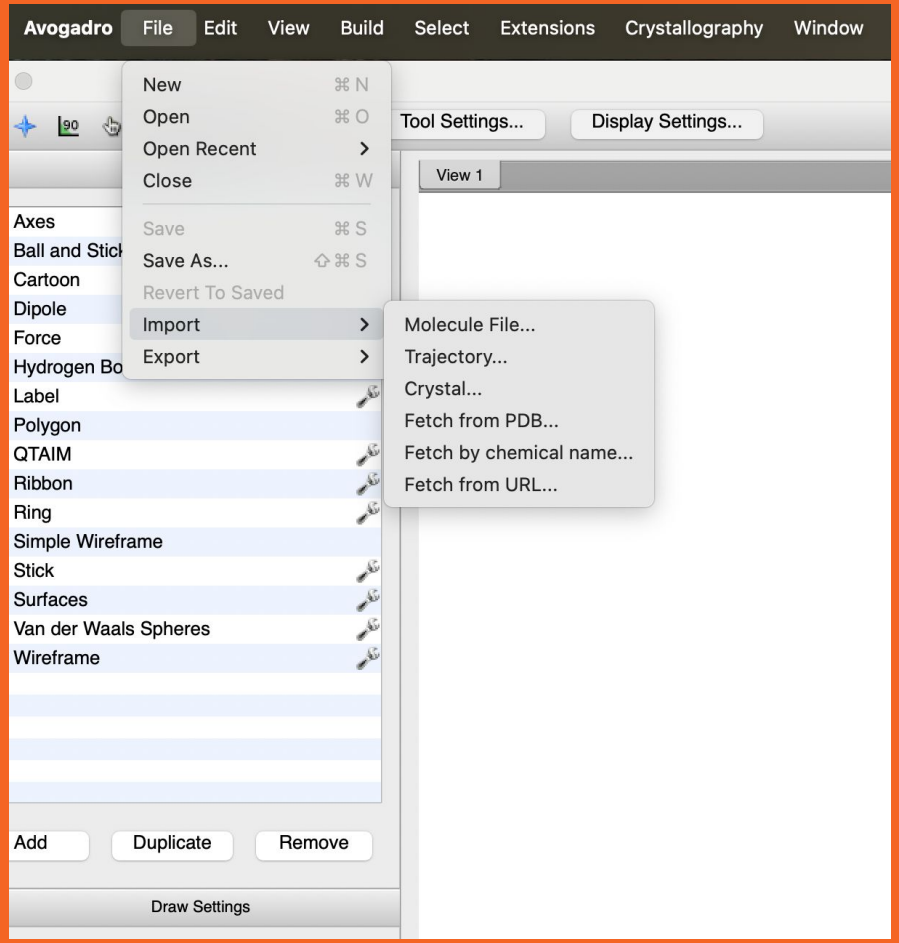




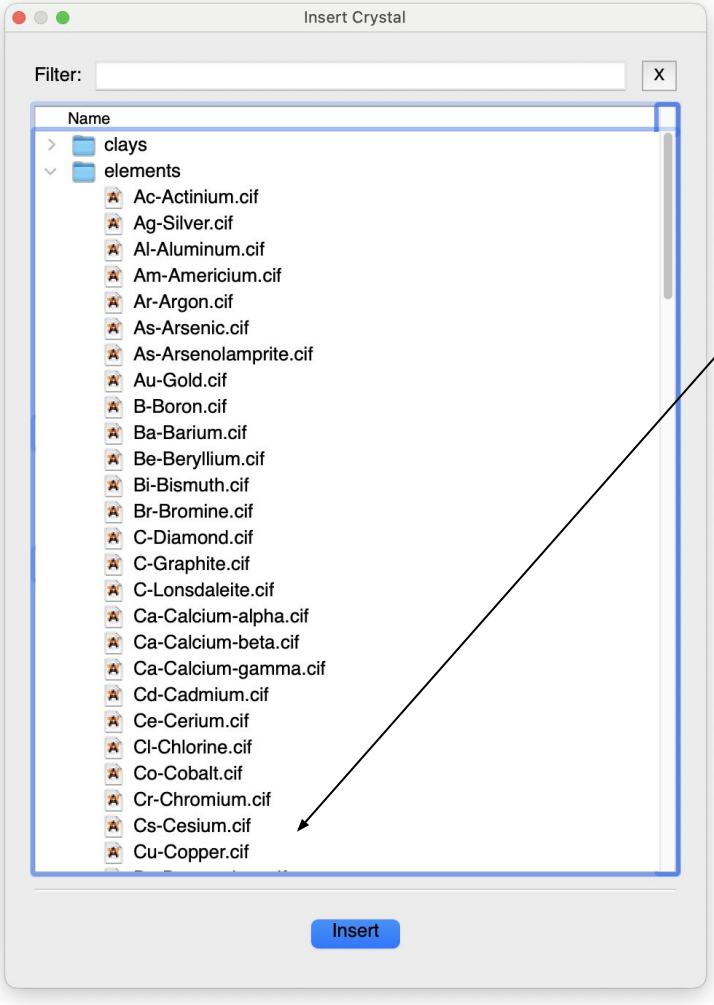
fcc conventional cell

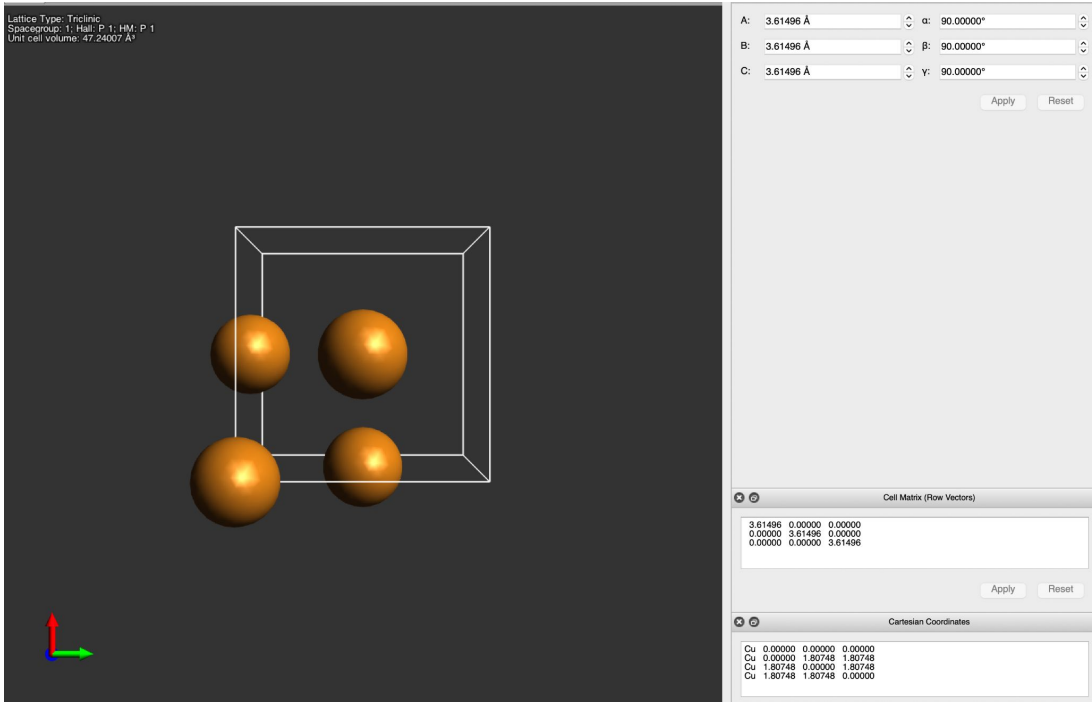
Avogadro

Step 1: Import a crystal

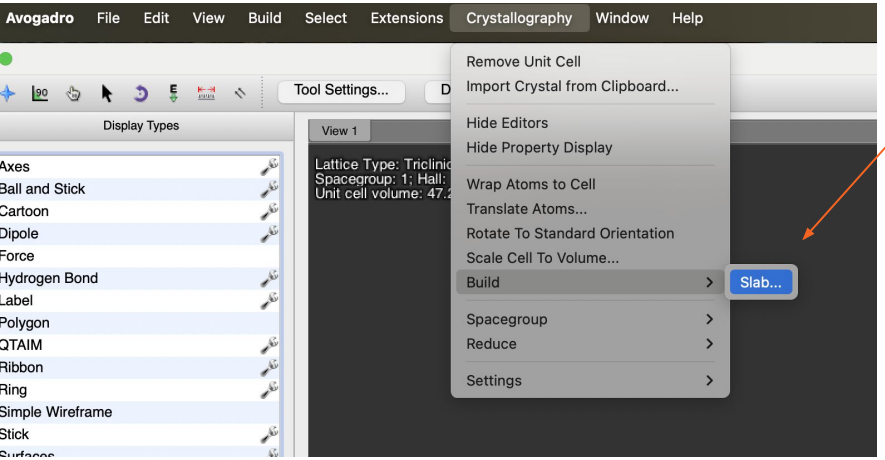


Step 1: Import a crystal - choose Cu

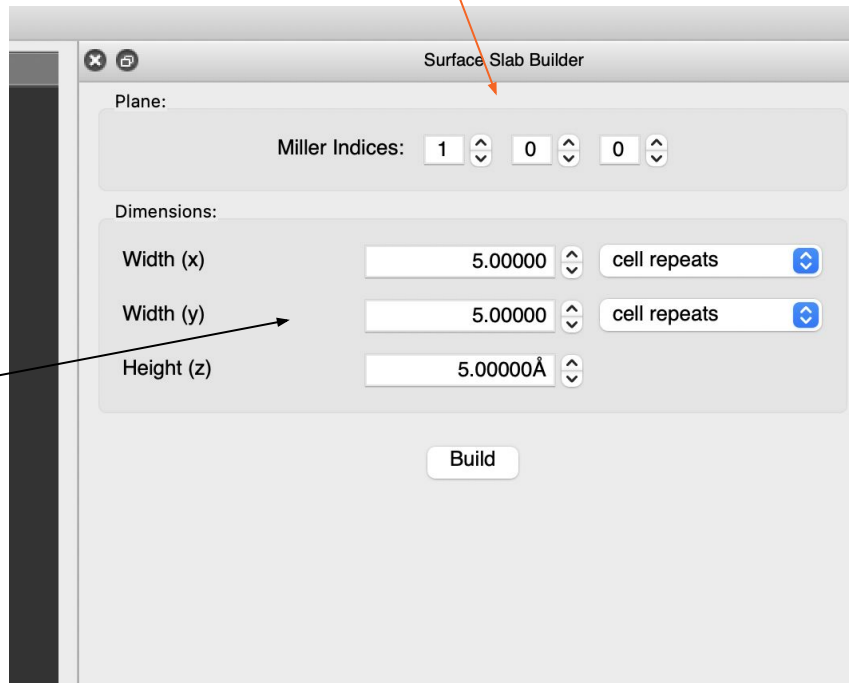




Step 2: Build the slab

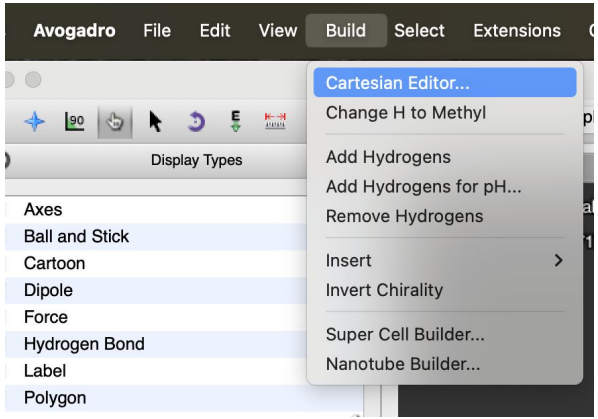


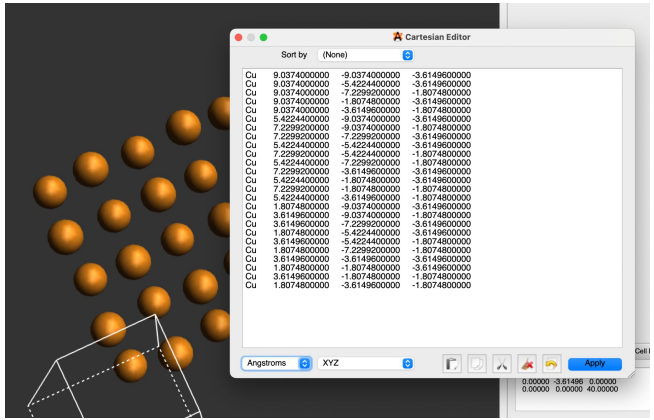
Step 3: Select what surface you want

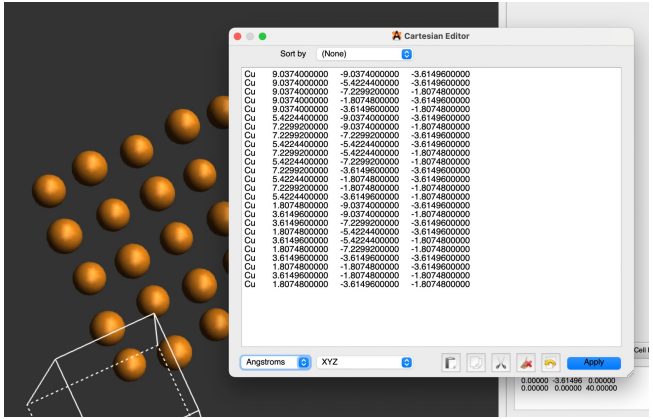


Step 4: Select the size

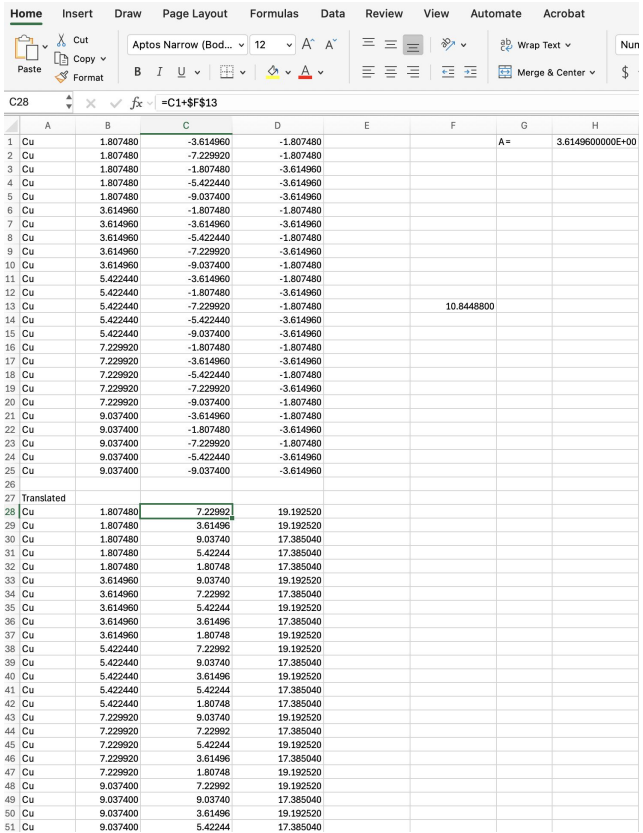
Step 5: Obtain the positions of the atoms, open cartesian editor







Step 6: Shift the atoms so they exist in the cell, open excel



Home Insert Draw Page Layout Formulas Data Review View Automate Acrobat

Paste Cut Copy Format Aptos Narrow (Bod... 12 Wrap Text Merge & Center

C28 =C1+F13

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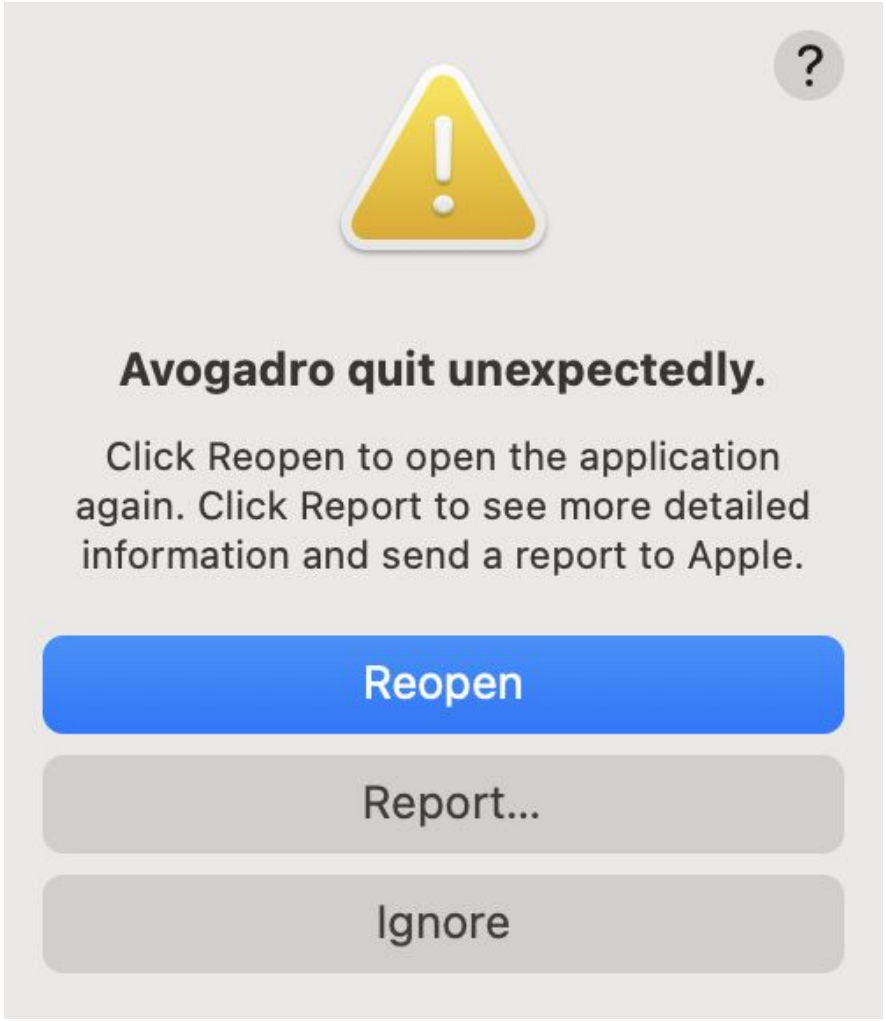
1	Cu	1.807480	-3.614960	-1.807480			A=	3.6149600000E+00
2	Cu	1.807480	-7.229920	-1.807480				
3	Cu	1.807480	-1.807480	-3.614960				
4	Cu	1.807480	-5.422440	-3.614960				
5	Cu	1.807480	-9.037400	-3.614960				
6	Cu	3.614960	-1.807480	-1.807480				
7	Cu	3.614960	-3.614960	-3.614960				
8	Cu	3.614960	-5.422440	-1.807480				
9	Cu	3.614960	-7.229920	-3.614960				
10	Cu	3.614960	-9.037400	-1.807480				
11	Cu	5.422440	-3.614960	-1.807480				
12	Cu	5.422440	-1.807480	-3.614960				
13	Cu	5.422440	-7.229920	-1.807480		10.8448800		
14	Cu	5.422440	-5.422440	-3.614960				
15	Cu	5.422440	-9.037400	-3.614960				
16	Cu	7.229920	-1.807480	-1.807480				
17	Cu	7.229920	-3.614960	-3.614960				
18	Cu	7.229920	-5.422440	-1.807480				
19	Cu	7.229920	-7.229920	-3.614960				
20	Cu	7.229920	-9.037400	-1.807480				
21	Cu	9.037400	-3.614960	-1.807480				
22	Cu	9.037400	-1.807480	-3.614960				
23	Cu	9.037400	-7.229920	-1.807480				
24	Cu	9.037400	-5.422440	-3.614960				
25	Cu	9.037400	-9.037400	-3.614960				
26								
27	Translated							
28	Cu	1.807480	7.22992	19.192520				
29	Cu	1.807480	3.61496	19.192520				
30	Cu	1.807480	9.03740	17.385040				
31	Cu	1.807480	5.42244	17.385040				
32	Cu	1.807480	1.80748	17.385040				
33	Cu	3.614960	9.03740	19.192520				
34	Cu	3.614960	7.22992	17.385040				
35	Cu	3.614960	5.42244	19.192520				
36	Cu	3.614960	3.61496	17.385040				
37	Cu	3.614960	1.80748	19.192520				
38	Cu	5.422440	7.22992	19.192520				
39	Cu	5.422440	9.03740	17.385040				
40	Cu	5.422440	3.61496	19.192520				
41	Cu	5.422440	5.42244	17.385040				
42	Cu	5.422440	1.80748	17.385040				
43	Cu	7.229920	9.03740	19.192520				
44	Cu	7.229920	7.22992	17.385040				
45	Cu	7.229920	5.42244	19.192520				
46	Cu	7.229920	3.61496	17.385040				
47	Cu	7.229920	1.80748	19.192520				
48	Cu	9.037400	7.22992	19.192520				
49	Cu	9.037400	9.03740	17.385040				
50	Cu	9.037400	3.61496	19.192520				
51	Cu	9.037400	5.42244	17.385040				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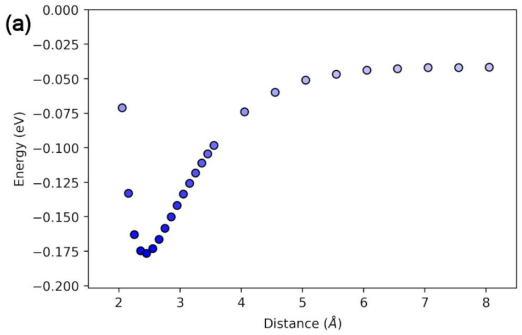
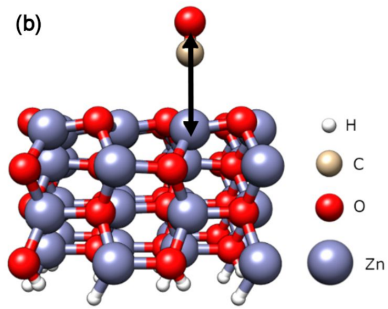
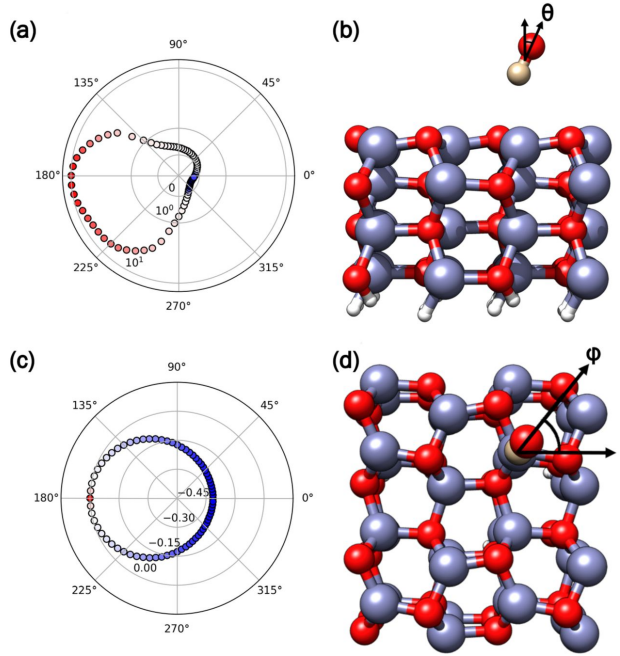
Report...
Ignore

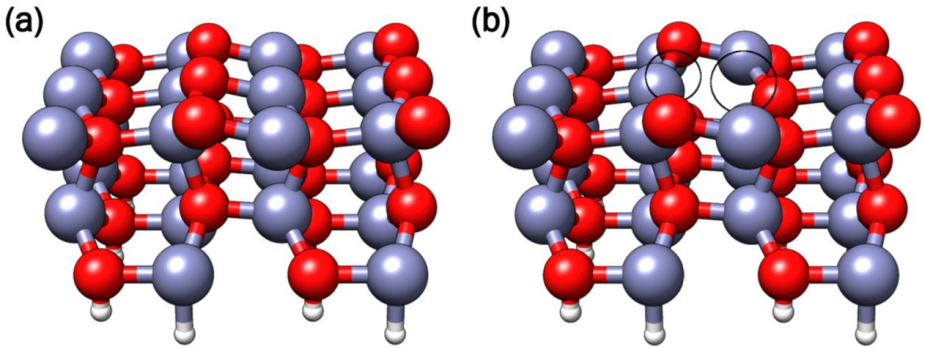






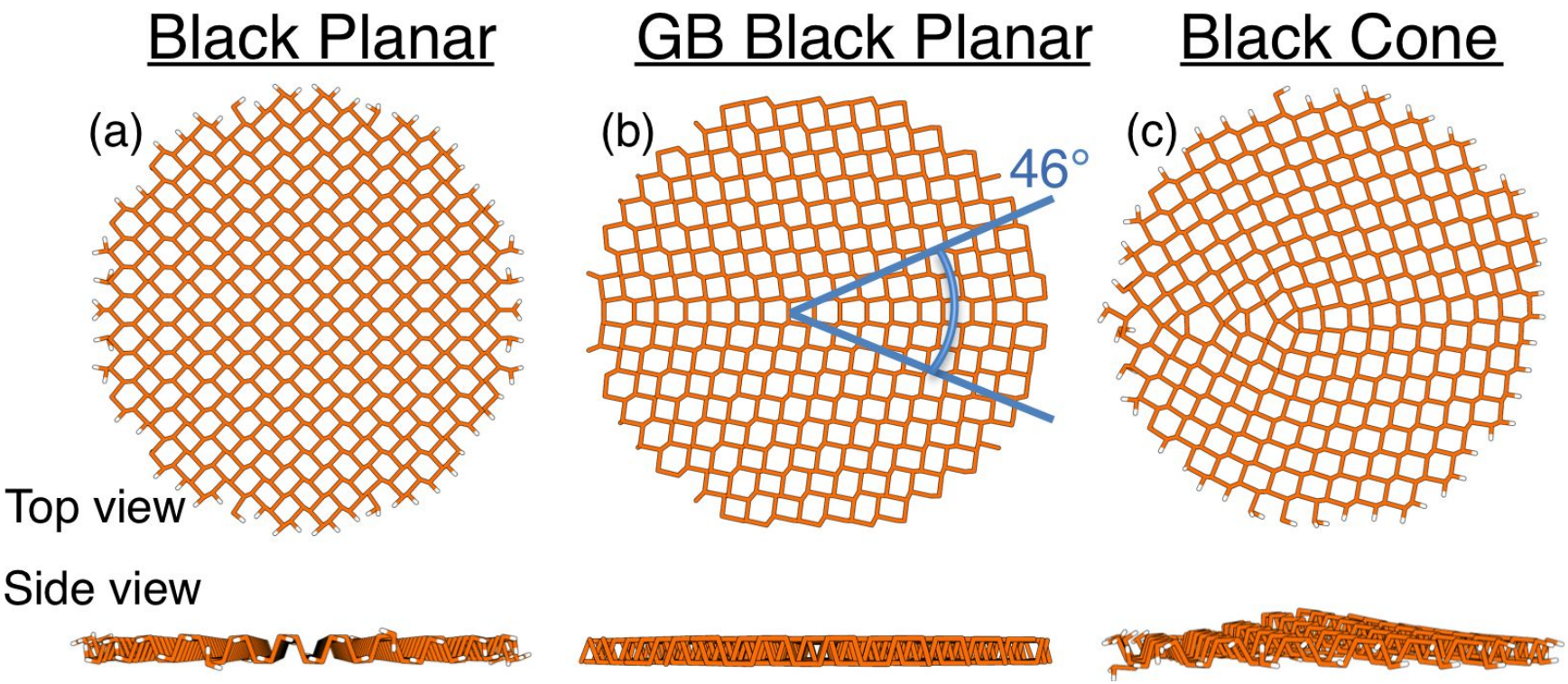
Theoretical Investigation of CO Adsorption on ZnO $(10\bar{1}0)$ and $(11\bar{2}0)$ Surfaces: The Role of Dimer Defects

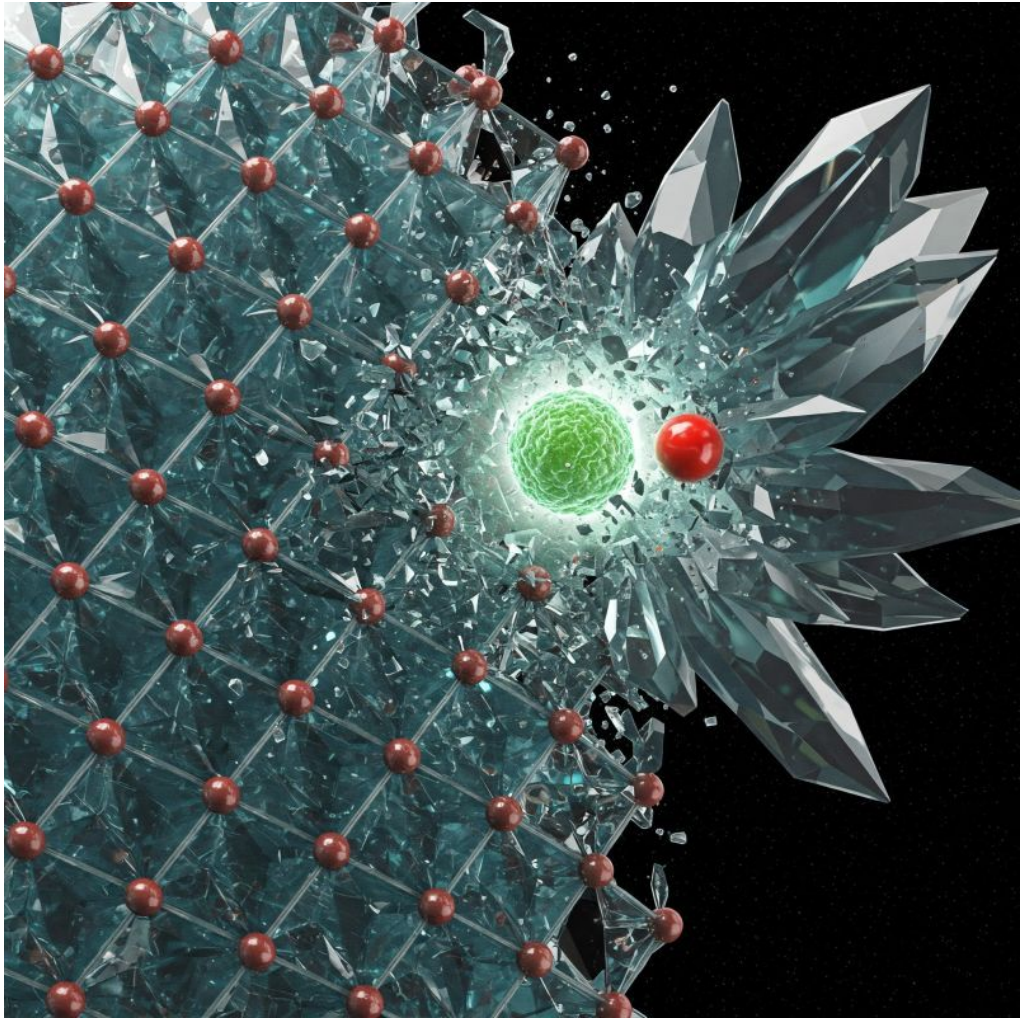
Kyle R. Stoltz and Mario F. Borunda*



Binding Energy: -2.6 eV ~ 60 kcal/mol

Black Phosphorus





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Threshold Displacement Energies in Lead Halide Perovskites from *Ab Initio* Molecular Dynamics Simulations

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Rosty B. Martinez Duque[1], Ahmad R. Kirmani[2], Ian R. Sellers[3], and Mario F. Borunda[1,4,*]

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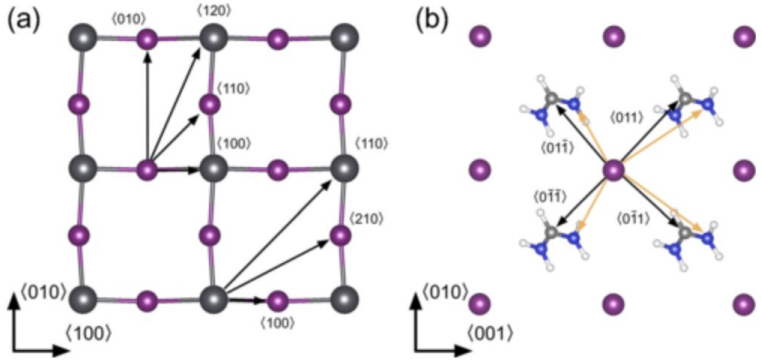

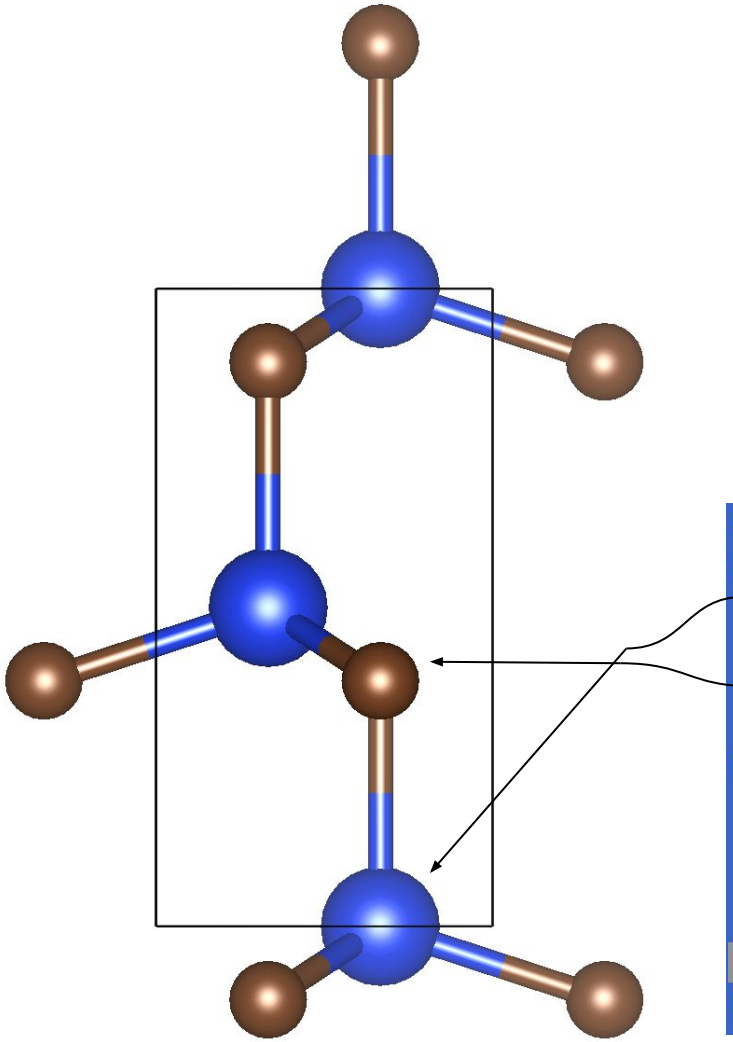

Change velocity in z-direction to: 1.0E-03 ~ 1.4 eV

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  2.9063895731E+00   1.6779983220E+00   8.4422716500E+00
:V(Bohr/atu):
 -3.2627960766E-05  -1.3242997933E-05   1.7796661557E-05
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  4.5317242924E-05  -1.8572714660E-05   1.8056426688E-07
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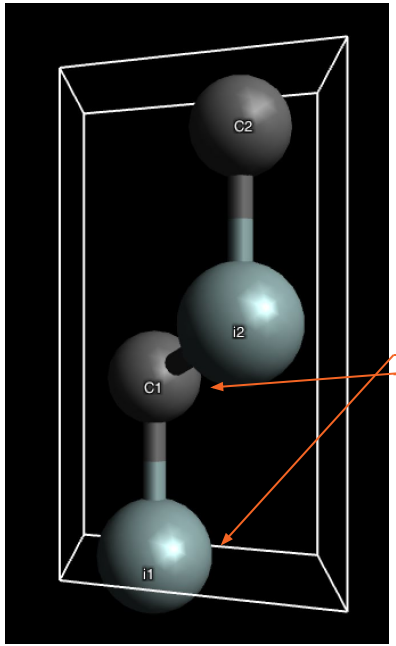


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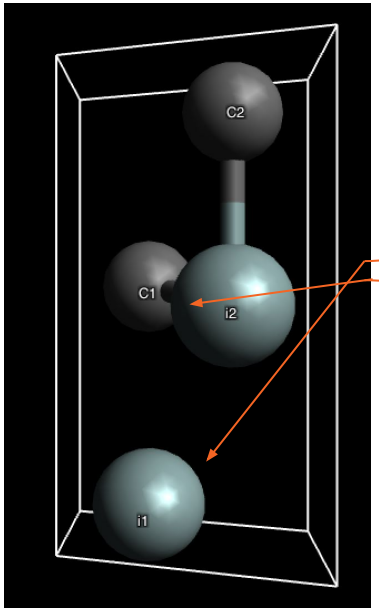


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```

This was the initial interaction, lasted for 50 fs
we need to monitor for 2 to 4 ps