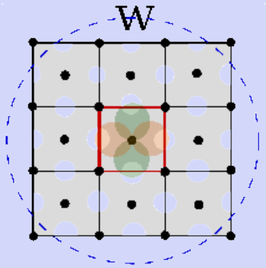
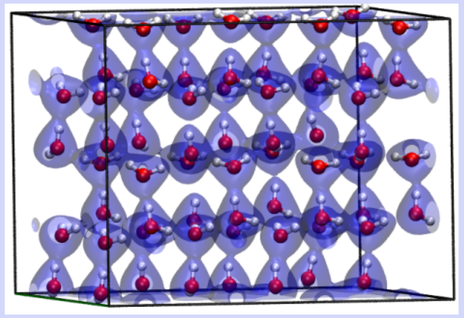
SALTED

rholearn

Learn Electronic Density



RI representation

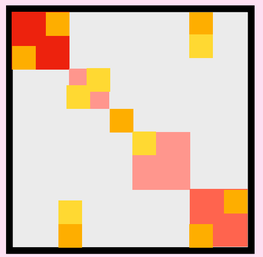


ACEHamiltonians.jl

DeepH

Learn Hamiltonian

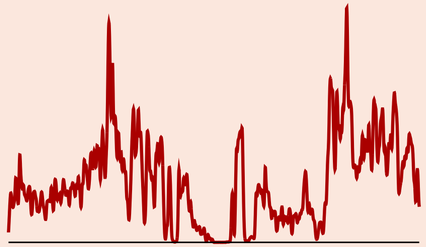
Atomic Simulation Interface



Numeric Atomic-Orbitals

FHI-aims

Raw outputs

doslearn

Learn Density of States etc.