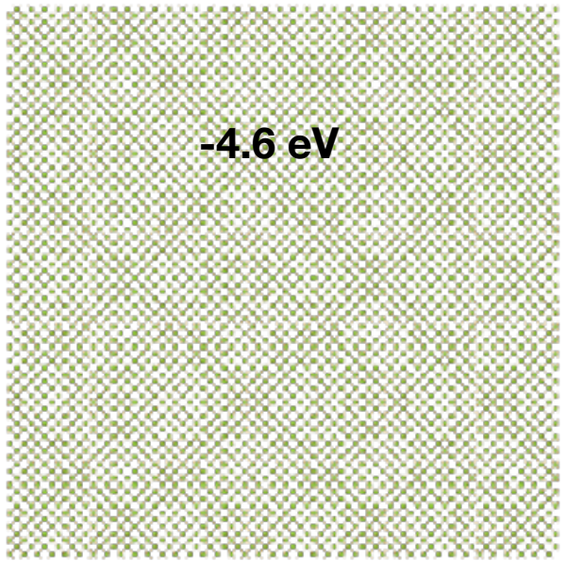
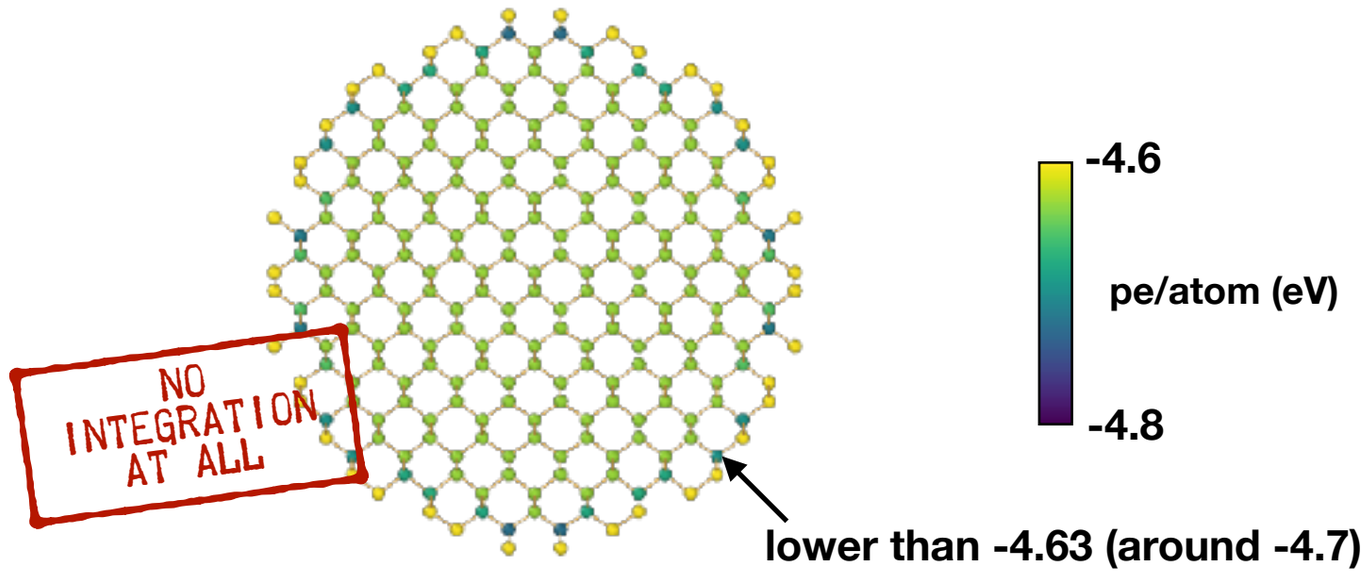
* initial energy check by LAMMPS with the Tersoff potential

just normal, no problem.



Cubic Diamond

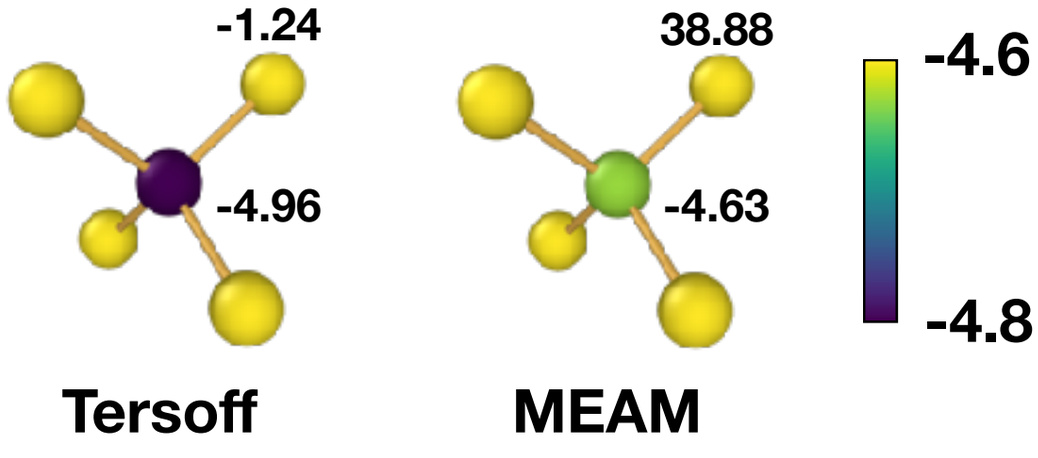
angles & pair distances are same,
initial energy must be identical with the diamond
except the far-most atoms which lack 4-fold bonds.



Nano-wire

nonetheless, strange atoms whose energy values
are much lower are found nearby the surface.

*isolated cubic diamond tetrahedron, initial energy check



it turns out there is some bug with the Tersoff
potential, a one-step lower energy value is found
with a simulation using a isolated tetrahedron.