

Questions

1. How to solve ImportError: No module named pybinding

I followed install steps in pybinding website. However all method I tried are useless.

2. How to add atom by using @pb.onsite_energy_modifier

I read a tutorial "Fields and effects", but I don't know how to add atom. I guess it require controlling onsite energy, but I don't understand it.

3. How to substitute atom

This is similar to Q-1. I guess this task require to adjust onsite energy and hopping energy, but I don't know how to adjust them.

4. What is hepta/penta defect, how to make it

I don't know what is hepta/penta defect, and how to make it

5. How to calculate DOS and LDOS, What is kernel polynomial method, how to use

I don't understand how to calculate DOS and LDOS. I don't know what is kernel polynomial method, and how to use it.