Computational Chemistry and Materials Modeling

Discussion of Lab 3 on Computational Chemistry of Crystals

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Questions to discuss

1. Modeling of layered crystals.
2. Other interesting discussions by students about their Lab 3.

Questions to discuss

Modeling of layered crystals

- There might be noncovalent interaction between layers (cf. graphene vs black phosphorus). In this case dispersion correction can be important.
- The direction perpendicular to the layer is often “soft” and should be scanned carefully (e.g. in volume scans). In particular, hexagonal setting is better than rhombohedral due to separation of “hard” and “soft” directions.
- Electronic structure might be a perturbation over single layer. In this case analysis of the electronic structure of the single layer is important.
- There might be interesting “phase transitions” when we change number of layers, e.g. metal-insulator, polymorphism.