

Computational Chemistry and Materials Modeling

Team project 3

Topic: materials

Formulate your own project within the above defined topic or do one of the following projects.

1. Evaluate KMnPO_4 as cathode material.
2. Evaluate polyfluorine as molecular donor in organic solar cells.
3. Evaluate possibility of creating a 2D As.
4. Study Si/ SiO_2 planar interface.
5. Study Si nanocrystals in SiO_2 .
6. Study reconstruction of Si surface.
7. Study SiO_2 polymorphs.
8. Study P polymorphs including molecules, polymers, and isolated layers.
9. Study Se polymorphs including molecules and polymers.
10. Evaluate stretching, bending, torsional strength of carbon nanotubes.
11. Characterize and compare mechanical/structural parameters of at least two different carbon nanotubes in the view of their possible application in structural composites.
12. Study intermolecular interactions in kevlar.

Reminder: This is a scientific project whose more or less complete solution has a complexity scale of a peer-reviewed publication. That is why a precise exhaustive solution is not required. But try to do your best, spending a reasonable amount of time (about 2 hours per week per team member). It is expected that you will take TA's advisory on team-projects. Prepare 10 min oral presentation (introduction, motivation, methodology, main results, conclusions) and be ready for additional 10 min of discussion. Very short written report is also required and should contain the information on participation of each team member.