

## Computational Projects

### Instructions

- (1) Select one of the following topics, or suggest your own, to be the topic for your computational projects.
- (2) Set up a meeting with the instructor to discuss your research plan (no later than April. 15) .
- (3) Work on your project under the guidance of the instructor.
- (4) A 10~15 minute presentation by end of this semester is required. The computational project will contribute to 30% of your final grade.

### Project list:

1. Use Buckyballs for hydrogen storage
2. Mechanical stability of graphene
3. Gas absorption on carbon nanotube tips
4. Structural configuration of BN nanotubes
5. Electronic structure of DNA molecules
6. The structure of methanethiolate on Ag (111)
7. Push a single Co atom on a copper surface
8. Chemisorption of CO on Cu(111)
9. Mechanical strength of Carbon Nanotube
10. Morphology study of small metallic clusters
11. Reactions of OH Radicals with Acetone in the Atmosphere
12. Ab initio calculations of the weakly bound cluster Ar-HCCCN
13. Ab initio calculation of protein-water interaction energies
14. Quantum mechanical energy optimization for protein-ligand structures
15. How does a gold nanowire break?
16. Structures and energetics of metal ion complexes in enzymes
17. Ab initio investigation of metal complexes
18. Structure and properties of oligomers
19. Simulation of liquid water near hydrophobic surfaces
20. First principle study of Borane and Al hydride clusters

Topics suggested by students are also permissible.