

## Topics for Term Paper

You can choose one of the following topics for your term paper. No restriction on length and format, but copy and paste from any resource is strictly prohibited, which will immediately leads to a fail of this course.

1. Recent progresses in post Hartree Fock quantum chemical methods
2. A new exchange-correlation functional in density functional theory
3. Wavelet based electronic structure calculation
4. Summary of methods to simulate a property of materials [choose a property not discussed in class]
5. Recent progresses in global optimization algorithm
6. Molecular simulation by combining MD and MC techniques
7. New methods for molecular simulation based free energy calculation
8. Machine learning in materials science