NST651 Computational Nanoscience: Electronic Structure Theory

Lecturer: Prof. Yong-Hyun Kim (yong.hyun.kim@kaist.ac.kr, Tel: 1111)

Text Book: Electronic Structure: Basic Theory and Practical Methods (Richard M. Martin)

Time: 9:30-11:00 AM, Monday and Wednesday, Fall, 2010
Place: Room 408, Creative Learning Building (E11)

Course Description: Computational simulation should be considered as a third means in modern research sciences, in addition to traditional methods like experiment and theory. For last two decades, the predicting power of computational nanomaterials science has been improved significantly owing to the rapid development of multiprocessors, parallel-computing linux clusters, and computational algorithms. From this class, you will learn methodologies of modern computational materials science and details of electronic structure theories, and also will perform a simple simulational research project using the state-of-the-art softwares such as VASP and PWscf.

Syllabus

Period	Contents	Period	Contents
Week 1	Introduction	**Week 9**	Exchange and correlation (Ch. 8)
Week 2	VASP and PWscf	**Week 10**	**Mid-term exam**
Week 3	Atoms and pseudopotentials (Ch. 11)	**Week 11**	Plane waves and basis sets (Ch. 12)
Week 4*	Molecules	**Week 12**	Total energy and electronic structure (Ch. 9)
Week 5	Solids (Ch. 4)	**Week 13**	Quantum molecular dynamics (Ch. 18)
Week 6	Nanomaterials (Ch. 2)	**Week 14**	Term project
Week 7	Uniform electron gas (Ch.5)	**Week 15**	Practice
Week 8	Density-functional theory (Ch. 6)	**Week 16**	**Final report and presentation**

*Happy Chuseok (no class): Sep. 22

Software:
- VASP: Commercial license. Okay to use during class. http://cms.mpi.univie.ac.at/vasp/.
- PWscf: Free. http://www.pwscf.org.

Hardware: Linux cluster supercomputer (machine name: kohn.kaist.ac.kr)

Evaluation: Attendance (30%), Practice (20%), Mid-term (10%), Final (40%)

Website: http://nano-bio3.kaist.ac.kr and click the Class menu
Questions? During/after class or Email me later.

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