Syllabus
高等计算固体力学/Advanced Computational Solid Mechanics
徐志平 (xuzp@tsinghua.edu.cn)

Lectures: 6 sessions, 3 hours / session
Requirements: solid mechanics, some quantum mechanics and statistical physics
For the in-class practice: laptop, registration for using FIT computational facilities

The textbook
[ZXB] Zhiping Xu, Xiaoyan Li, and Bin Liu, *Atomistic Simulations Methods in Solid Mechanics*, Tsinghua University Press (*manuscript in preparation*)

Suggested readings
[AT] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Oxford University Press, 1989. ISBN: 0198556454. (*general reference*)
[FS] D. Frenkel and B. Smit, *Understanding Molecular Simulation: From Algorithms to Applications, 2nd Ed.*, Academic Press, 2001. ISBN: 0122673514. (*for free energy methods)*
[R] D. C. Rapapport, *The Art of Molecular Dynamics Simulation*, Cambridge University Press, 1998. ISBN: 0521599423. (*for transport properties calculations*)

Grading
4 weekly assignments
1 final project assignment

Week 1 (10 Sep)
Lecture 01 – An introduction
Mechanics of materials, microstructures of materials, some solid state physics

Week 2 (17 Sep)
Lecture 02 – Basic molecular dynamics simulations
Numeric methods, forcefield, analysis and visualization of results
MD step by step

Week 3 (24 Sep)
Lecture 03 – Intermediate molecular dynamics
Coupling to the environments, temperature & pressure, transport

Week 4 (8 Oct)
Lecture 04 – Advanced molecular dynamics
The length & time scales, free energy calculations

Week 5 (15 Oct)
Lecture 05 – Extending molecular dynamics
Potential development, quantum effects

Week 6
Lecture 06 – Applications of molecular dynamics