PKU Globex Julmester®

The Materials Genome Assessment (3 Credits)

材料基因组评估

Instructor	**Cedric WEBER**, Physics, King's College London, UK (cedric.weber@kcl.ac.uk)		
Synopsis	This course provides a pedagogical introduction to computational modeling. Computational modelling is used in a wide range of applications, such as material science, bio-medical engineering, finance, etc. In particular, scientific modeling can be used to accelerate the discovery of new materials (The so-called "materials genome" project): nowadays, simple physical equations are implemented in computer software, enabling researchers to carry out "virtual" experiments with predictive capabilities. The course will provide the students with an awareness of the importance of material discovery and its societal impact, and during hands-on sessions we will provide the students with a tutorial for *Materials Studio*, a modern computational tool suite. The course will consist of both lectures and practical sessions in the computer room. We will also have discussion sessions and group work, where material discovery is discussed in the wider context.		
Offering	2018 Julmester (July Semester)		
Audience	Undergraduate and Graduate Students (all majors and all levels) with no prerequisites		
Classroom	Room TBA, Teaching Bldg. No. TBA, Peking University		
Schedule	Class: 1-4 PM, M-F, July 2–20, 2018	Final Exam: No Exam	Total Contact Hours: 45
Objective	To develop an understanding of the fundamental components of computational modelling and its application to materials and molecules. During the first part of the course, we aim at providing the students with an awareness of the importance of materials discovery, its societal impacts, and provide an introduction to some exotic state of matter such as super-conductors or low-dimensional materials, such as graphene. We will also provide an introduction to "materials genomics". During the second part of the course, the aim is to provide a pedagogical introduction to some very simple but important computational algorithms, such as Monte Carlo and how to solve differential equations (with little or no knowledge of the mathematics). We will then discuss some of the most advanced quantum modelling techniques (so-called density functional theory) and classical modelling approaches (so-called molecular dynamics), which can be applied to materials discovery. The course will focus on both the theory and its applications, and a tutorial to the computational suite *Materials Studio* will be given during hands-on session.		
Topics	1. Materials discovery to meet the challenges of the 21st century 2. What is computational modeling, and how can it be used to investigate the "materials genome" 3. Monte Carlo 4. Hands-on: computing the value of Pi by using game theory 5. How to solve differential equations with little knowledge of the mathematics 6. Hands-on: explaining the breakdown of the Tacoma bridge 7. Strategies to guide materials design with software engineering 8. Introduction to *Density functional theory* and its application to material discovery 9. A tool suite to model materials: *Materials Studio* 10. How to predict the structure of a material 11. Time evolution with molecular dynamics 12. Hands-on: Carbon nanotubes 13. Quantum computing and quantum information 14. How to predict colors: optical absorption and quantum mechanics 15. Superconductors and their applications 16. A single atomic sheet of atoms: Graphene		
References	1. D.P. Landau, A guide to Monte Carlo simulations in statistical physics, Cambridge Univ. Press, 3rd edition (2009) 2. D. Sholl & J.A. Steckel, Density functional theory: a practical introduction, John Wiley § Sons. Inc. London (2011) 3. D. Frenkel & B. Smit, Understanding Molecular Simulations, Academic Press (2001) 4. Other articles provided by instructor.		
Grading	Small Group Project Presentation 1 30% Small Group Project Presentation 2 30% Mid-Term Exam 30% Attendance and Participation 10% **Total 100%**		