MATE130053	计算材料学	学分：2	周学时：2
	Computational Materials Science	总学时：36	
预修课程：	近代物理（量子力学）		
修读对象：	主要面对大四学生，大三学生和留学生亦可选		

中文课程简介（150 字以内）

本课程介绍利用计算机来模拟、理解和预测真实材料性质的基本知识。主要内容包括密度泛函理论下的电子结构和分子动力学计算、基于 GW 近似的能带结构计算、传输性质计算等。目的是使学生对材料性质的第一原理计算有一定基本了解、能够欣赏计算材料学的最新进展并在将来工作需要时能自己进行一些常规的模拟计算。

英文课程简介

This course is designed to provide students basic knowledge on computer simulations to model, understand, and predict the properties of real materials. Specific topics include: density functional theory and the total-energy pseudopotential method; geometry optimization and molecular dynamics; band structure calculation and GW approximation; transport properties. The course employs case studies of advanced materials and nanotechnology. In the lecture, basic theory will be interwoven with hand on tutorial for codes and step by step practical instruction. The ultimate goal is to provide students with basic knowledge on computational materials and to elevate students to a level where they can appreciate modern work on materials property calculation and can carry out a first principle calculation by themselves.