学术报告

题　目： **What Quantum Mechanical Calculations Can Do For You**

报告人： **Prof. Graeme Ackland**

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时　间： **2015 年 1 月 21 日(周三)上午 09:00**

地　点： **中科院固体所新楼 520 会议室**

摘要：

In this talk, Prof. Ackland will briefly describe what is and isn't possible using calculational techniques based on electronic structure calculations and molecular dynamics. He will concentrate on the areas where experimental and computational input are both essential to obtaining an understanding of the material in question. He will not attempt a detailed explanation of the tricks and pitfalls involved in solving the quantum mechanics, but will describe in more detail two pieces of work. The first is the determination of the structure and dynamical properties of Hydrogen at high pressure, in particular the so-called "Phase IV". This has been identified only in spectroscopy experiments and in theoretical calculations. Together, these present a picture of a complicated crystal structure in which the molecule are on the verge of stability. The low symmetry structure is a way of lowering the free energy of the material, and avoiding metallization.

His second application is more practical - he will show how under titanium alloys can be designed to be machinable. The problem for most titanium alloys is that when cut the waste material forms a long, unbroken, spiral chip which eventually clogs up the machine. It then required expensive and time consuming manual intervention to remove the chip. He describes molecular dynamics and electronic structure calculation at very high stresses, such as found in a cutting experiment. He will show how the phase structure can be made to self-organised into a region with very high temperature and commensurately low shear strength during machining. This then causes the cut material chip to break off. This allows us to design an alloy which is easy to use in manufacturing, but retains its normal properties when recovered to ambient conditions.

报告人简介：

Ackland 教授于英国牛津大学获博士学位后到英国 Harwell 原子能研究院工作，曾在美国宾州大学从事博士后研究，2003 年起任爱丁堡大学计算模拟教授，2006 年任该校凝聚态和复杂系统研究所所长。他在第一原理计算领域开展过开拓性工作，主要贡献包括：参与了第一原理软件包 CASTEP 的早期开发，以该主题发表的 50 多篇论文被引用超过 2000 次；他构建的 Fe 及其它过渡金属的原子间作用势被广泛应用于分子动力学模拟，相关论文被引用 1500 余次；他开发并维护的分子动力学软件 MOLDY，在世界范围内得到广泛应用。Ackland 教授在材料科学领域的工作包括高压相变、核材料、马氏体相变及钛、镍合金切削加工的计算模拟。他研究兴趣广泛，曾建立计算模型模拟进化与兴起过程、动物集中畜群、新石器时代农业、经济发展与危机模式等复杂系统。Ackland 教授在 *Science, Nature Materials, PNAS, Phys Rev Lett* 等期刊发表论文 150 多篇。