北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Seminar

Computer Modelling as a Tool in Materials Science

Richard Catlow

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Time: 4:00pm, July 4th, 2016 (Monday)

时间：2016年7月4日 （周一）下午4:00

Venue: Room W563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

Computer modelling techniques are now used very widely in chemical, physical and biological sciences, especially in understanding the behaviour of complex systems at the molecular level. This lecture will highlight their application to materials science where the impact has been substantial in recent years. Special emphasis will be given to six important and topical areas:

•Crystal structure prediction
•Guiding and understanding synthesis
•Modelling defects and Ion transport
•Modelling nucleation and growth
•Understanding reactivity at the molecular level
•Modelling structures and properties of nano-particles

Applications to oxides, microporous silicates sulphides and molecular crystals will be discussed. Future prospects and developments in the field will be considered.

About the speaker

Prof. Charles Richard Arthur Catlow is a Professor in the Department of Chemistry, University College London. He became a Fellow of the Royal Society (FRS) in 1990. Since then, he played an important role in the Royal Society, and took many important positions such as the Chair of Royal Society sub-committee 3 (Chemistry), the member of the Council of the Royal Society, etc. His current work is centred around the investigation of complex materials using a combination of computer modelling, quantum mechanical, synchrotron radiation and neutron scattering techniques. He has co-authored or edited 15 books. His citation is over 34,000 and his H–Index is 89.