南開大學化學學院
COLLEGE OF CHEMISTRY NANKAI UNIVERSITY

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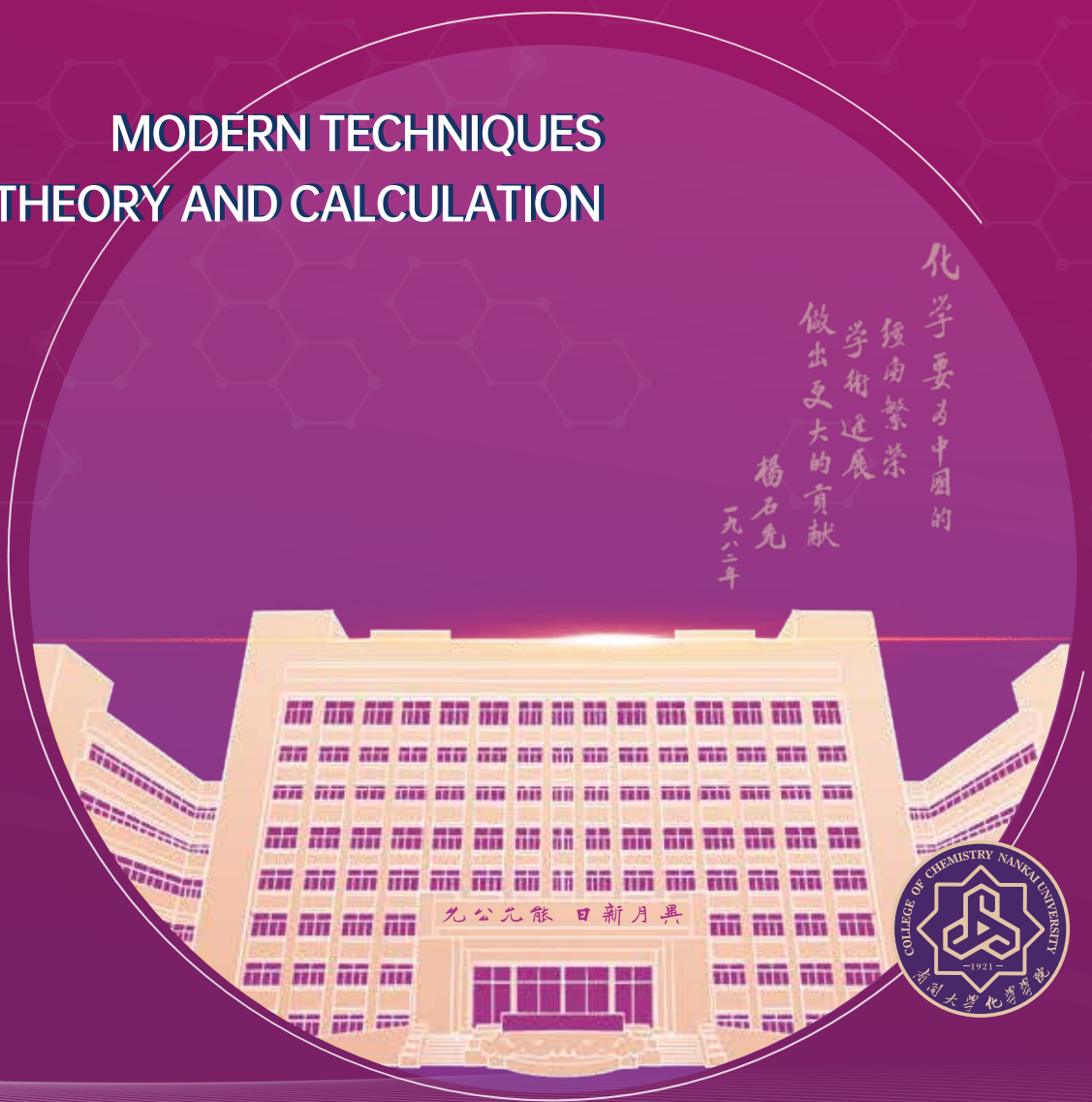
（现代理论与计算技术）

化学及交叉学科前沿-南开峰会
理论与计算化学专场

MODERN TECHNIQUES IN THEORY AND CALCULATION



MODERN TECHNIQUES IN THEORY AND CALCULATION

6月8日

PROFESSOR CHRIS SKYLARIS
(University of Southampton, UK)

16:00

报告题目

LARGE-SCALE QUANTUM ATOMISTIC ELECTROCHEMISTRY SIMULATIONS

(大规模量子学原子电化学模拟)

简介

Professor C. Skylaris, is from Department of Chemistry, University of Southampton. He is currently working on development of large-scale quantum chemistry and multiscale simulations methods, motivated by the need to provide solutions to challenging chemistry problems such as new materials, catalysis and drug design.

Chris-Kriton Skylaris studied Chemistry at the National and Kapodistrian University of Athens in Greece and received a first class MChem degree in 1996. He received a PhD in Quantum Chemistry from the University of Cambridge in 1999. Following an EU ICARUS Fellowship at the CINECA supercomputing centre in Bologna in Italy, he carried out postdoctoral research in the Theory of Condensed Matter group at the Cavendish Laboratory at the University of Cambridge, till 2004. He has held a Royal Society University Research Fellowship from 2004 till 2012, first at the University of Oxford and then at the University of Southampton. In 2006 he was appointed to a Lectureship in Chemistry at the University of Southampton. Chris is currently a Professor of Computational Chemistry and Director of Programmes.

研究领域

Chris's research focuses on the development of theory, algorithms and codes for quantum mechanical (QM) calculations from first principles on parallel computers. He is a founding and leading author of the ONETEP program for large-scale (linear-scaling) quantum chemistry simulations. Many of the developments are incorporated into the ONETEP program which is also used by other researchers in academia and industry.

网址

网址：https://www.southampton.ac.uk/chemistry/about/staff/cks.page

PROFESSOR JONATHAN YATES
(oxford university, uk)

17:00

报告题目

UNDERSTANDING THE STRUCTURE OF MATERIALS USING COMPUTATIONAL AND EXPERIMENTAL NMR

(使用计算和实验NMR了解材料的结构)

简介

Associate Professor of Materials Modelling, University of Oxford

研究领域

Jonathan's research lies in the field of computational electronic structure theory. In brief, it is the development of new theoretical methods, their implementation into easy to use computer packages, and finally their application to novel scientific problems.

A major theme of his research has been the development of computational methods to interpret solid-state Nuclear Magnetic Resonance (NMR) experiments. Applications have included pharmaceutical compounds, (bio)minerals and glasses.

Further work has involved the development of techniques to interpret Electron Energy Loss Spectroscopy (EELS) with applications to nano-structured materials and interfaces.

Other work has focused on the use of so-called Wannier functions (www.wannier.org) to describe the properties of metallic systems: Fermi surface properties, transport, phase transitions etc.

This research has led to two publicly available codes: Castep www.castep.org for spectroscopic properties and Wannier90 www.wannier.org to obtain wannier functions.

网址

网址：https://www.materials.ox.ac.uk/peoplepages/yates.html

MODERN TECHNIQUES IN THEORY AND CALCULATION

6月9日

JOSEPH BARKER
(University of Leeds, UK)

18:00

报告题目

ATOMISTIC SPIN DYNAMICS WITH A QUANTUM THERMOSTAT

(量子热浴原子自旋动力学)

简介

Joseph Barker obtained his PhD at the University of York. He then took a position as an assistant professor in the Theoretical Physics Group of the Institute for Materials Research, Tohoku University in Japan. He moved to Leeds in 2018 as a Royal Society University Research Fellow.

My group's research is into magnetic materials and their applications, specialising in the modelling of magnetic materials using large scale computer simulations, calculating the thermodynamic and dynamical behaviour, including non-equilibrium behaviour and phase transitions. We aim to perform quantitative calculations of materials for technological or experimental applications. We have developed an in-house atomistic spin dynamics package over 10 years which has been GPU accelerate from the beginning. Our recent interests have been in insulator spintronics, studying materials such as yttrium iron garnet. We have also been trying to make methodological advances to include more quantum effects in our calculation to make results quantitatively accurate across temperature ranges.

研究领域

Main research is into magnetic materials and their applications, specialising in the modelling of magnetic materials using large scale computer simulations, calculating the thermodynamic and dynamical behaviour, including non-equilibrium behaviour and phase transitions.

网址

网址：https://eps.leeds.ac.uk/physics/staff/5729/dr-joseph-barker

MARTINA STELLA
(Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy)

19:00

报告题目

A NOVEL TRANSITION-BASED CONSTRAINED DFT (TCDFT) FOR THE ROBUST AND RELIABLE TREATMENT OF PURE AND MIXED EXCITATIONS IN MOLECULAR SYSTEMS

(用于处理分子系统中的纯激发及混合激发的一种新型稳定的跃迁约束DFT (TCDFT))

简介

Senior Research Fellow at ICTP. Modelling the electronic structure of molecular systems and materials by developing multi-scale methods (QM/QM, QM/MM) to achieve high accuracy with reduced computational cost.

研究领域

Martina is a computational physical-chemist with an interest in modelling the electronic structure of molecular systems and materials by developing multi-scale methods (QM/QM, QM/MM) to achieve high accuracy with reduced computational cost. Her current interest is developing a methodology for an accurate and computationally sustainable description of excited states in extended systems and materials (e.g TADF materials) in the linear-scaling DFT code, BigDFT. She also uses DFT for applications and collaborations with experimental groups in the field of surface chemistry and mechanochemistry.

In recent years she started working with classical molecular dynamics for modelling the tribology of lubricants in confined and extreme conditions, e.g. under shear and high pressure

网址

网址：https://www.ictp.it/research/cmsp/members.aspx

MODERN TECHNIQUES IN THEORY AND CALCULATION

6月10日

MICHAEL HERBST
(RWTH Aachen University, Germany)

16:00

报告题目

BLACK-BOX ALGORITHMS AND ROBUST ERROR CONTROL FOR DENSITY-FUNCTIONAL THEORY

(密度泛函理论的黑箱算法和鲁棒误差控制)

简介

Applied and Computational Mathematics (ACoM), RWTH Aachen University.

研究领域

Research revolves around the quantum-chemical modelling of atoms, molecules and solids. He is in particular interested in developing efficient and reliable algorithms for the regime of high-throughput screening calculations in the solid state.

网址

网址：https://michael-herbst.com/research/

NICK HINE (university of warwick, uk), READER

17:00

报告题目

MACHINE LEARNED INTERATOMIC POTENTIALS FOR THEORETICAL SPECTROSCOPY OF MOLECULES IN SOLVENT ENVIRONMENTS

(机器学习原子间势用于研究溶剂环境中分子理论光谱)

简介

Department of Physics, University of Warwick.

He is an Associate Professor (Reader) in the Theory Group in the Department of Physics. My research involves theory and simulation of nanomaterials. I am a developer of

the ONETEP Linear-Scaling Density Functional Theory Package, which enables us to perform realistic simulations of large systems comprising thousands of atoms. This allows us to study complex systems such as proteins, heterostructure interfaces, layered materials, molecular crystals, and semiconductor nanocrystals.

He is a member of the UKCP Consortium, a High-End Consortium for access to the ARCHER supercomputer, and I am a member of the CCP9 Working Group, and PI of the current CCP9 Flagship Project. I am also a major user of Warwick's local HPC facilities, via the Scientific Computing Research Technology Platform, and the ATHENA system of the HPC Midlands Plus.

研究领域

Research involves theory and simulation of nanomaterials; A developer of the ONETEP Linear-Scaling Density Functional Theory Package.

网址

网址：**https://www.york.ac.uk/physics/people/probert/**

MODERN TECHNIQUES IN THEORY AND CALCULATION

6月10日

PROFESSOR MATT PROBERT

(University of York, UK)

19:30

报告题目

RAPID AB INITIO MD THROUGH ON-THE-FLY TRAINING OF GAUSSIAN APPROXIMATION POTENTIALS FROM DFT

(通过DFT高斯近似势的On-The-Fly算法训练快速从头算分子动力学)

简介

Department of Physics, University of York.

Matt leads the Condensed Matter Dynamics group which is part of the Condensed Matter Physics group. His research is focused on the application of computer modelling to understanding the properties of materials. CASTEP is a widely used general purpose materials modelling computer program based upon Density Functional Theory. It is developed by a team of UK Academics of which Matt Probert and Phil Hasnip are two of the leading authors. He is the Director of N8 Centre of Excellence in Computationally Intensive Research and Chair of UKCP.

研究领域

QC Physics-DFT, Path Integral Molecular Dynamics, Genetic algorithms, Materials simulation, ab initio calculations, CASTEP.

网址

网址：https://www.york.ac.uk/physics/people/probert/

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