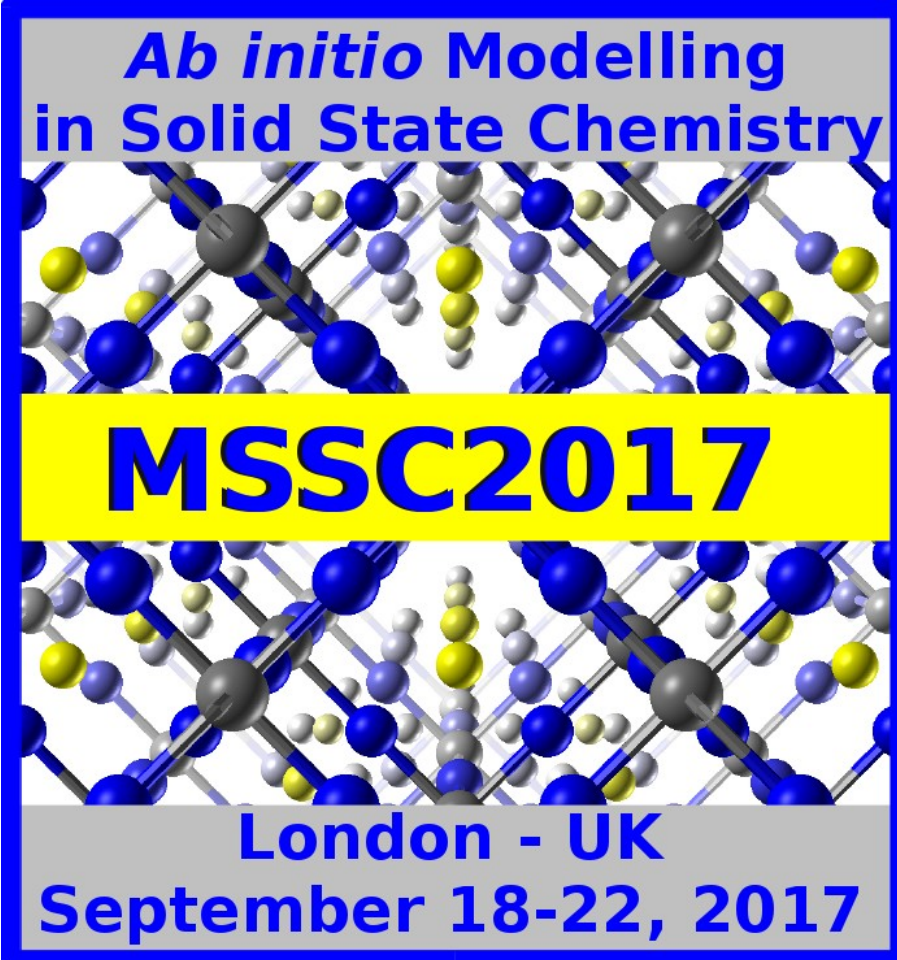

WORKSHOP REPORT



Ab initio Modelling
in Solid State Chemistry

MSSC2017

London - UK
September 18-22, 2017

<http://www.imperial.ac.uk/mssc2017/>

Abstract

The Department of Chemistry and the Thomas Young Centre at Imperial College London and the Computational Materials Science Group of the Science and Technology Facilities Council (STFC), in collaboration with the Theoretical Chemistry Group of the University of Torino, organised the 2017 MSSC Summer School on the "*ab initio* modelling of crystalline and defective solids with the CRYSTAL code".

The school provided an overview of the underlying theory and fundamental issues affecting use of the CRYSTAL code, with particular emphasis on practical issues in obtaining reliable data efficiently using modern computer hardware.

The capabilities of CRYSTAL was illustrated with hands-on tutorials organized in the afternoon sessions.

All information about the school can be found on this website:

<http://www.imperial.ac.uk/mssc2017/>

Attendees

Speakers

- Ehsan Ahmad - Imperial College London (UK)
- Maria L. Alfredsson - University of Kent (UK)
- Leonardo Bernasconi - STFC Rutherford Appleton Laboratory, Oxfordshire (UK)
- Ian J. Bush - Oxford e-Research Centre, University of Oxford (UK)
- Gerit Brandenburg - University College London (UK)
- Silvia Casassa - Università di Torino (Italy)
- Furio Corà - University College London (UK)
- Alessandro Erba - Università di Torino (Italy)
- Andrea Ferretti - S3 Center, Istituto Nanoscienze, CNR, Modena (Italy)
- Nic M. Harrison - Imperial College London (UK)
- Giuseppe Mallia - Imperial College London (UK)
- Ruth Martínez - Imperial College London (UK)
- Lorenzo Maschio, Università di Torino (Torino)
- Barry G. Searle - STFC Daresbury Laboratory (UK)

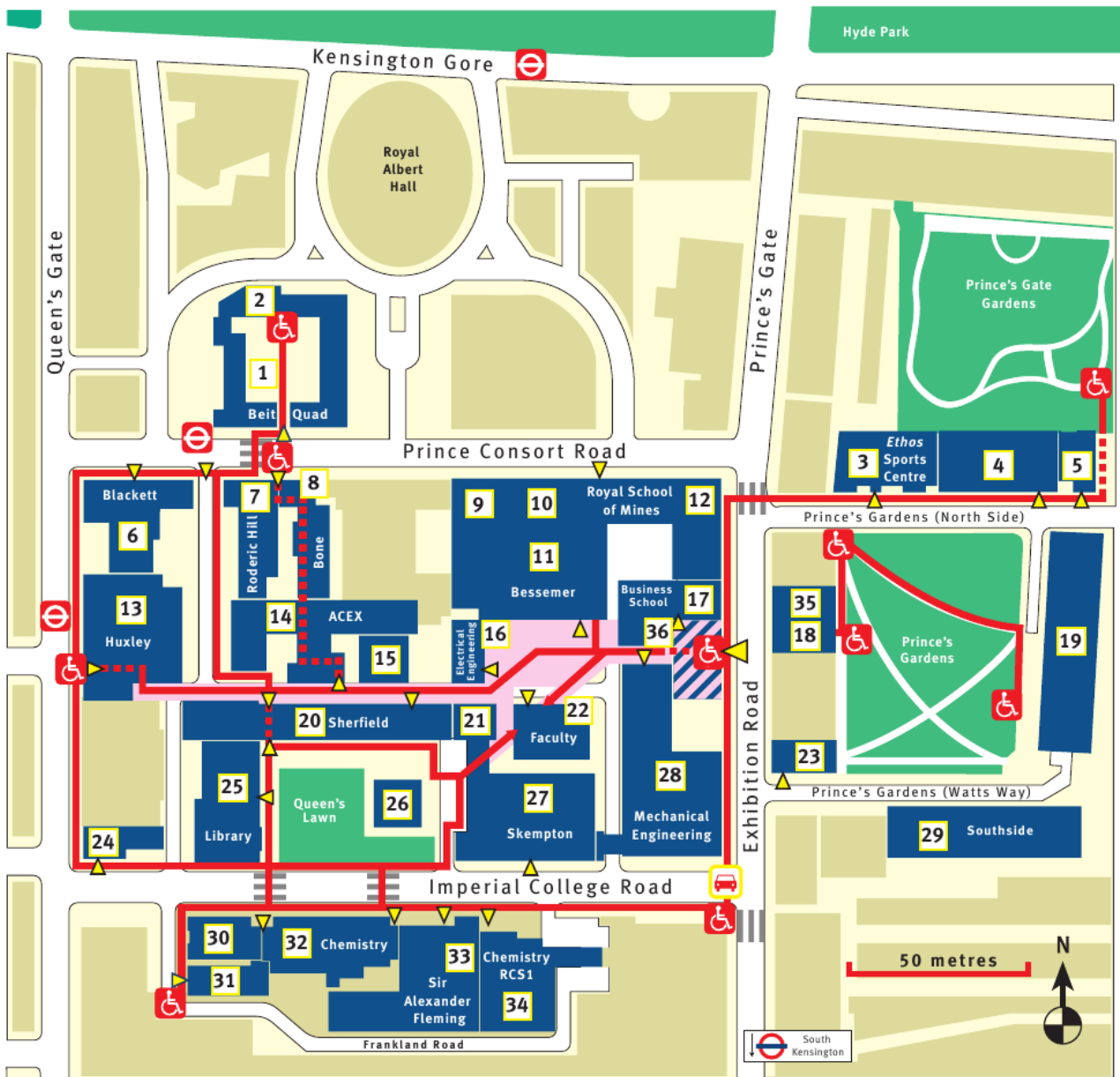
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Location

MSSC2017 took place from Monday 18 – Friday 22 September at...

- **Registrations and Morning Sessions - Royal School Of Mines, Prince Consort Rd, Kensington, London SW7 2BP (Building 12)**
- **Afternoon Sessions - Department of Chemistry/Biochemistry, South Kensington Campus, London SW7 2AZ (Building 32)**



Programme

MORNING SESSIONS: RSM - Room 1.31

Coffee Break: Royal School of Mines (RSM) / Department of Materials - Room 1.31

	Monday 18th	Tuesday 19th	Wednesday 20th	Thursday 21st	Friday 22nd
9:00 - 9:45	Translation symmetry, space groups, Bloch functions, Fermi energy G. Mallia	The structure of the CRYSTAL code G. Mallia	Local defects in crystalline materials G. Mallia	Localized crystalline orbitals and related quantities L. Bernasconi	Modeling low-dimensional systems with CRYSTAL: Nanotubes and Fullerenes S. Casassa
9:45 - 10:30	Quantum Chemical Methods L. Bernasconi	Quasi-harmonic Approximation: Thermal Effects on Structural and Thermodynamic Properties A. Erba	Vibrational frequencies calculation and tools for their analysis L. Maschio	Post-HF techniques and the CRYSCOR project L. Maschio	Dielectric and optical properties of solids L. Bernasconi
	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>	<i>Coffee Break</i>
10:50 - 11:35	Density-functional theory L. Bernasconi	The effect of pressure: equations of state; bulk modulus; elastic constants M. Alfredsson	Infrared and Raman Spectra of Solids L. Maschio	CRYSCOR: studied cases R. Martinez-Casado	Excited states. TD-DFT L. Bernasconi
11:35 - 12:20	Geometry optimisation of solids A. Erba	One-electron properties F. Corà	Ab initio thermodynamics E. Ahmad	Dispersion-corrected mean-field electronic structure methods G. Brandenburg	Quantum transport in nanojunctions A. Ferretti
12:20 - 13:05	CRYSTAL input/output. Basic features. Scripts. G. Mallia	From bulk to surface. Relaxation and reconstruction. G. Mallia	CRYSTAL in parallel I. Bush	TOPOND: topological analysis of the electron charge density of solids S. Casassa	Predictive simulation and materials characterisation N. Harrison

AFTERNOON SESSIONS: Chemistry/Biochemistry Building

Coffee Break and Poster Session: Department of Chemistry
Chemistry Cafe' (Room 232)

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BASIC TUTORIALS : ROOM 311 - BIOCHEMISTRY BUILDING

	Monday 18th	Tuesday 19th	Wednesday 20th	Thursday 21st	Friday 22nd
14:30 - 16:15	Geometry input	DLV: visualisation of structures and properties. B. Searle Total energy (Single-point)	13:05 - 15:45 <i>Lunch & Poster Session</i>	Vibrational frequencies	Nanotube systems
	<i>Coffee Break</i>	<i>Coffee Break</i>		<i>Coffee Break</i>	<i>Coffee Break</i>
16:45 - 18:30	Basis set input & basis set editing	Geometry optimisation	16:00 ... <i>Self-guided Tour</i>	One-electron properties. TOPOND: electron density analysis	Basic modelling of surfaces and defects

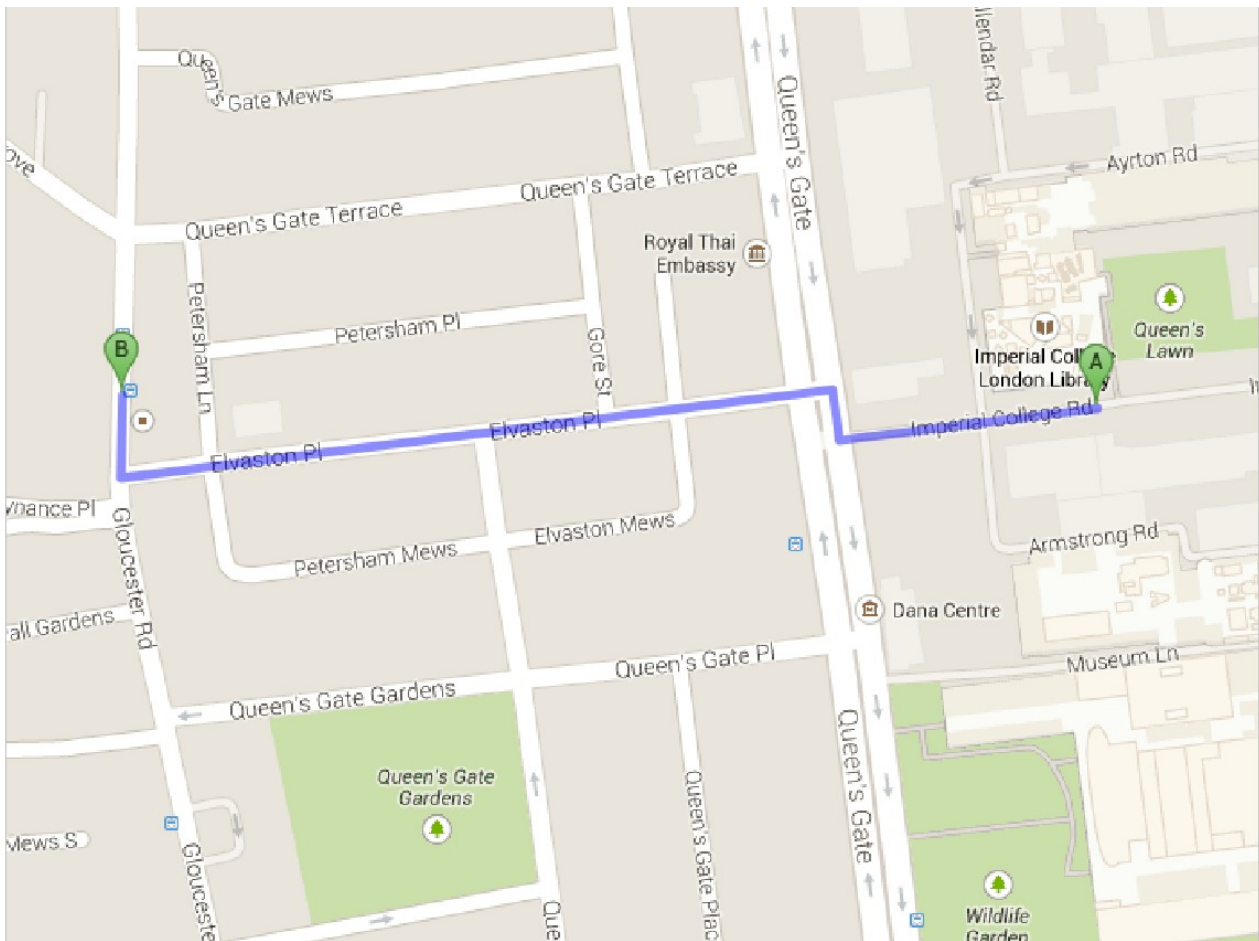
ADVANCED TUTORIALS : ROOM 310 - BIOCHEMISTRY BUILDING

	Monday 18th	Tuesday 19th	Wednesday 20th	Thursday 21st	Friday 22nd
14:30 - 16:15	Advanced options in geometry optimisation and frequencies calculation	Magnetic properties	13:05 - 15:45 <i>Lunch & Poster Session</i>	CRYSTAL in Parallel Mode: Pcrystal vs. MPPcrystal	Dielectric properties
	<i>Coffee Break</i>	<i>Coffee Break</i>		<i>Coffee Break</i>	<i>Coffee Break</i>
16:45 - 18:30	Advanced options in geometry optimisation and frequencies calculation	Magnetic properties	16:00 ... <i>Self-guided Tour</i>	CRYSOR	Dielectric properties

Social Dinner

The MSSC Dinner took place on Wednesday 20 September at...

MED KITCHEN RESTAURAN
25–35 Gloucester Road
London SW7 4PL



Tutorial Session



Some Feedback

- 1) This is a very good conference. I will recommend it. Thank you!
- 2) The tutorial sessions were very helpful! I had a very nice time.
- 3) Content is well organised. Excellent practice work.
- 4) For the most part, the speakers were very good at helping to understand the topics and gave clear explanation of how things works and why the methods are used.
Social dinner was good and food was yummy.
Poster session was good and it was nice to see a wide range of topics and where people want to apply CRYSTAL. Thanks you for putting on this workshop, it has been very useful and educational in helping improve my understanding of not only CRYSTAL, but of DFT and HF code in general. I feel that I have learnt a lot from this and have thoroughly enjoyed it.
- 5) A good balance of various topics and of types of talks (technical, general and applications). Excellent workshop! I enjoyed the talks and tutorial. A job well done :-)
- 6) Tutorial sessions: Wonderful!
- 7) I was very satisfied with the workshop overall. It was much more useful than what I have expected, since I got answers to many questions that were unclear only from the program manual. Thank you.
- 8) Basic tutorial were incredibly helpful and well structured. It was easy to follow all the steps. Thanks for all the help, material and information provided.
- 9) Social dinner was a wonderful experience for me, to get to know lots of people.