



We would like to draw your attention to the forthcoming 21<sup>st</sup> WIEN2k workshop to be held at Nantes (France) from Weds 2<sup>nd</sup>- Sat 5<sup>th</sup> July, 2014. In connection, we will organize an international conference on advanced materials modelling (ICAMM-2014) open to all codes, from Mon 7<sup>th</sup>- Weds 9<sup>th</sup> July, 2014.

The registration fee is significantly reduced for participants attending both meetings. Additionally these two events are supported by the Psi-k network, **as a consequence 20 to 30 scholarships supporting student participation will be available.**

**March 15, 2014:** Short abstract submission deadline for ICAMM 2014 conference, student bursary application deadline.

**April 15, 2014:** Notification to the authors of the acceptance and mode of presentation of their communications for ICAMM 2014 conference.

**May 15, 2014:** Early fee registration deadline, extended abstract submission deadline for both meetings.

**June 15, 2014:** Registration deadline.

More details are available at <http://www.cnrs-imn.fr/ICAMM2014>

### WIEN2k WORKSHOP July 2-5, 2014

The 21<sup>st</sup> workshop in the history of the WIEN code is a hands-on activity dedicated to teaching the use of the WIEN2k Density Functional Theory Package. WIEN2k is one of the most popular electronic structure codes used to perform calculations with the Full Potential LAPW method. The workshop is a unique opportunity to learn the use, power and limitations of the package with the tutoring of the authors and developers of the code. The activities will be aimed at graduate students and researchers from industry and academia. The only pre-requisite is to have a basic knowledge of solid state physics, and chemistry. It is planned as a five-day activity with lectures on the scientific aspects of the method, applications, hands-on activities on selected examples. It is a unique opportunity to receive a head start on a personal project.

#### The workshop covers three aspects:

- Introduction to DFT and FLAPW methods
- Applications using WIEN2k code (and related methods)
- Lectures on and exercises with WIEN2k

### ICAMM 2014 *3<sup>rd</sup> edition of the International Conference on Advanced Materials Modelling* July 7-9, 2014

This is the third edition of a bi-annual conference gathering scientists from the fields of theoretical chemistry and physics, who are interested in:

- Using calculations to understand the properties of advanced materials (optical, electronic, magnetic, ferroelectric, piezoelectric, multiferroic, catalytic, photovoltaics), with applications in energy storage and conversion, memories, optoelectronics...
- Code developments (WIEN2k, VASP, FHI-AIMS, CASTEP, ABINIT, SIESTA, Quantum ESPRESSO, OCTOPUS, AIMPRO ...) and new implementations in semi-empirical and/or first-principles approaches
- Spectroscopic simulation (XAS, ELNES, VEELS, XPS, IR/Raman, NMR ...).

### Chairs:

- **Florent Boucher**, IMN, France
- **Chris Ewels**, IMN, France
- **Xavier Rocquefelte**, IMN, France

### Scientific Committee:

- **Peter Blaha**, TU Vienna, Austria
- **Stefano Baroni**, Scuola Internazionale Superiore di Studi Avanzati (SISSA) Trieste, Italy
- **Gerbrand Ceder**, Massachusetts Institute of Technology, USA
- **Xavier Gonze**, Université Catholique de Louvain, Belgium
- **Jean-François Halet**, Sciences Chimiques de Rennes, France
- **Chris Pickard**, University College London, United Kingdom
- **Angel Rubio**, Facultad de Químicas, Universidad del País Vasco, Spain
- **Isao Tanaka**, Kyoto University, Japan
- **Philippe Sautet**, ENS Lyon, France

### Location:

The Institute of Materials ([www.cnrs-immn.fr](http://www.cnrs-immn.fr)) is located in the beautiful city of Nantes ([www.nantes-tourisme.com](http://www.nantes-tourisme.com)). Nantes is the 6<sup>th</sup> largest city in France, situated on the Atlantic coast, south of Brittany.

### Confirmed invited speakers (ICAMM conference):

**Prof. Sharon Ashbrook**, University of St Andrews, UK

*Development of new methods in solid-state NMR, first-principles calculations of NMR parameters in the solid state*

**Prof. Bertram Batlogg**, ETH Zürich, Switzerland

*Creating and understanding materials and their novel physical phenomena (high temperature superconductors, quantum magnets, oxide superconductors, heavy fermion compounds, mixed-valence compounds...)*

**Dr. Elena Bichoutskaia**, University of Nottingham, UK

*Theoretical and Computational Chemistry (carbon nanomaterials, van der Waals forces, gas storage...)*

**Prof. Régis Gautier**, Institut des Sciences Chimiques de Rennes, ENSCR, Rennes, France

*Bonding and structure-properties relationships, solid-state NMR parameters*

**Prof. Frank de Groot**, Utrecht University, Netherlands

*Synchrotron and Theoretical Spectroscopy of Catalytic Nanomaterials*

**Dr. Anubhav Jain**, Lawrence Berkeley National Laboratory, Berkeley, USA

*The Materials Project: A Public Materials Database*

**Prof. Steven G. Louie**, University of California at Berkeley, USA

*Theoretical condensed matter physics and nanoscience (quasiparticle and optical excitations, reduced-dimensional systems, superconductivity; ab initio pseudopotential theory; topological insulators...)*

**Dr. Lucia Reining**, École Polytechnique, Palaiseau, France

*Many-body theory and first principles calculations of electronic excitations and spectroscopy (ETSF)*

**Dr. Oleg Rubel**, Lakehead University, Thunder Bay, Canada

*Berry phase in WIEN2k, piezoelectrics for therapeutic ultrasound, optoelectronics...*

**Prof. Gotthard Seifert**, Technische Universität Dresden, Germany

*Quantum Chemistry, Cluster Physics & Chemistry and Computational Materials Research*