AB INITIO MODELLING OF ADVANCED MATERIALS (AMM 2019)

DECEMBER 8, 2019 | YURI GORNOSTYREV | LEAVE A COMMENT

Workshop Ab initio Modelling of Advanced Materials (AMM 2019)

10-13 September 2019, Onegin hotel, Ekaterinburg, Russia

From 10th to 13rd September 2019 the second workshop AMM2019 devoted to the recent progress in the development and application of ab-initio based methods of calculation and thermodynamic/kinetic modeling for microstructure and finite-temperature properties of a wide range of materials was held at conference hall of Onegin hotel in Ekaterinburg, Russia. This workshop welcomed 73 participants from 14 countries (including organizers), and 3 staff members. During the workshop, 25 oral talks and 14 key-note lectures were presented. The event was sponsored Psi-k organization, and the Institute of Metal Physics Ural division RAS (Ekaterinburg, Russia).

The purpose of this workshop was to brings together prominent scientists from the area of theoretical modelling to assess the state of the art in applications of the electronic structure theory for the knowledge-based design of advanced materials. Because the AMM2019 workshop was scheduled as a satellite to the international conference on magnetism EASTMAG-2019, the cooperation-promoting atmosphere of the both events were provided. The special topic of AMM2019 was related to problems of magnetism and magnetic materials. The main focus of the AMM2019 was to provide a fruitful framework for development and dissemination of novel ideas and concepts in order to resolve the present challenges in the field and development of new strategy for design of the materials by using combined multi-disciplinary efforts.

For the contemporary advanced materials, a proper account for magnetic effects as well as for correlation effects in electronic structure and thermal excitations is also an important and quite challenging problem. Therefore, the workshop encompasses (i) accurate computational methods that are able to capture phenomena at the electronic and atomic level, (ii) efficient coarse-graining methodologies to access microstructure and target physical properties determined by micro and mesoscales and (iii) application of these approaches to the advanced materials. During the conference, a short AMULET hands-on on practical calculations of the physical properties of real materials will take place.

The workshop was articulated along three main tracks: magnetism and magnetic materials (1st day), strongly correlated materials (2nd day), advanced materials I and II (3rd and 4th days). A fairly representative poster session (24 contributions) was held at the end of the first day and the master class "Application of the AMULET code for DFT+DMFT calculations of realistic compounds" took place at the end of the second day of workshop. The key-note lectures opened each (morning and afternoon) Section and were followed by the oral presentations. The following lectures cause of special interest (see presentations):

Olle Eriksson, Attila Szilva, Uppsala University, "Spin-lattice simulations; formalism and some initial results"

Tamio Oguchi, Osaka University, "Materials Design of Heusler Alloys for Spintronics"

Sergey Savrasov, University of California Davies, "Weyl semimetals"

Ryotaro Arita, T. Nomoto, The University of Tokyo, "Anomalous transverse transport and domain wall motion in non-collinear antiferromagnets"

Luca de' Medici, Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris "Electronic compressibility and high-Tc superconductivity: new links"

Leonid Pourovskii, CPHT-Ecole Polytechnique, "Multipolar superexchange interactions and low-temperature ordered phases in actinide dioxides"

Eva Pavarini, Forschungszentrum Jülich, "Spin-orbit effects and magnetism in strongly correlated t2g materials"

Malte Rösner, Radboud university, Nijmegen, "Competition of strong charge and spin fluctuations in monolayer NbS2"

Ivan Leonov, Institute of Metal Physics, Ekaterinburg, "Interplay of electronic structure, magnetic state and lattice stability in iron oxides under extreme conditions"

Tilmann Hickel, Halil Sözen, Fritz Körmann, Jan Janssen, Jörg Neugebauer, MPIE, Dusseldorf, "Ab initio based finite temperature phase stabilities of hard-magnetic materials"

Vladimir Mazurenko, Ural Federal University, Ekaterinburg, "Neural network approaches for material science and quantum computing"

Alexander Lichtenstein, University of Hamburg, "Electron correlations in Magnetic and Superconducting Materials"

Tony Paxton, King's College, London, "Microscopic origins of plastic anisotropy in magnesium"

Igor Solovyev, S. Nikolaev, NIMS, Tsukuba, Tokyo Institute of Technology, "Electric polarization induced by skyrmionics order in GaV4S8: from first- principles calculations to microscopic models"

Organizers

The organizers of this school were:

- Yuri Gornostyrev (Ekaterinburg, Russia)
- Mikhail Katsnelson (Nijmegen, Netherlands)
- Joerg Neugebauer (Dusseldorf, Germany)
- Vladimir Anisimov (Ekaterinburg, Russia)

The local organizers from Ekaterinburg were:

- Nadezhda Gornostyreva
- Iliya Lomaev
- Inna Frolova

Conclusions and prospects

This workshop was successful in many ways: the number of participants, high level of lectures and presentations, warm working atmosphere, and participants responded very positively and contributed with their energy and enthusiasm.

Because of the enthusiastic response of participants, it was decided to reiterate this event in a couple of years (Sept. 2021, preliminary), trying to cover new and more advanced and hot topics in ab initio modeling field.

Further details

[Event website, with program and list of participants](#)

[Full program, with abstracts](#) and [presentations](#)

[Full list of participants](#)