DS 38: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Friday 10:30–12:45   Location: HL 001

DS 38.1   Fri 10:30   HL 001

Ab initio photoluminescence in 2D materials — ●Pedro Melo[1,4], Andrea Marini[2,4], Matthieu Verstraete[1,4], and Zeila Zanolli[3,4] — [1]NanoMat / CESAM, ULiege Belgium — [2]ISM CNR, Italy — [3]RWTH Aachen Germany — [4]ETSF

The theoretical study of photoluminescence (PL) has been hindered in the past due to lack of predictive ab initio numerical techniques [1,2,4]. We present a complete theoretical framework for the computation of PL where electrons, nuclei, and photons are quantised. The intrinsic non-equilibrium nature of the process is fully taken into account [3]. Starting from the Keldysh contour, we arrive at a set of equations for the Green's functions of electrons, phonons, and photons where the different kinds of interactions are treated on the same footing. These equations are then simplified by using the generalised Baym-Kadanoff ansatz and the completed collision approximation [3]. This reduces the problem to a set of decoupled equations for the density matrix that describe all kinds of static and dynamical correlations. We show how the micro-macro connection relates the observable spectrum with the time-dependent microscopic dynamics, via the Bethe-Salpeter equation. Finally, we present the results of our numerical studies on 2D materials, such as WS2, where we relate the evolution of the carrier populations in the Brillouin zone with the changes in the PL spectrum of the material, for a range of experimental setups. [1] M. F. Pereira and K. Henneberger, PRB 58, 2064 (1998). [2] K. Hannewald, et al, PRB 67, 233202 (2003). [3] P. M. M. C. de Melo and A. Marini, PRB 93, 155102 (2016). [4] S. W. Koch, et al, Nat Mat 5, 523 (2006).

DS 38.2   Fri 10:45   HL 001

Strain on molybdenum disulfide sheets with defects from first principles — ●Mohammad Bahmani[1], Mahdi Faghihnasiri[2], and Thomas Frauenheim[1] — [1]BCCMS, Physics Department, Bremen University, Bremen, Germany — [2]Physics Department, Shahrood University of Technology, Shahrood, Iran

Single layer of transition metal dichalcogenides(TMDCs) are under intense investigations since the discovery of unique characteristics of 2D and Vann der Waals layered materials. They are predicted to be the most promising structure for various future nanoscale devices. They have also novel applications in spintronic and optoelectronic. As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which show significant effects on their electrical, optical, vibrational, magnetic, and chemical properties. Besides, mechanical strain has very much influence on the electronic properties of 2D materials, particularly TMDCs. For example, 0.5% biaxial strain force direct band gap in molybdenum disulfide(MoS2) to become indirect since it breaks the crystalline symmetry. Therefore, I study different types of point defects such as single and double sulfur(S), single molybdenum(Mo) vacancies, and removing a Mo with its three upper S neighbors. I also substitute a Mo vacancy with one and two S atoms. Furthermore, as the second aim of this study, I showed the modification of defect states under uniaxial and biaxial compression and tensile strain. For the case of one S vacancy, this moves shallow states into the valance band and importantly breaks the degeneracy of degenerate states.

DS 38.3   Fri 11:00   HL 001

Competion of magnetic interactions and in-field behavior of cycloidal Uranium compound UPtGe. — ●Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Stimulated by recent high-field experiment [1] performed on unique actinide system with cycloidal magnetic structure, UPtGe, I performed a series of calculations aiming to understand the nature of the sequence of magnetic phase transitions caused by the applied magnetic field. The physics of the system is determined by the fine balance of the exchange interaction, magnetic anisotropy, and Dzyaloshinskii-Moriya interaction. This balance of interactions governs, in particular, the in-field behavior of the system. The physical consequences of the vari-

ation of the localization of the U 5f electrons is investigated.
[1] A. Miyake, A. Nakamura, Y. Shimura, Y. Honma, D. Li, F. Honda, M. Tokunaga, D. Aoki, doi.org/10.11316/jpsgaiyo.71.1.0_2062.

DS 38.4   Fri 11:15   HL 001

Electron correlation effects in the electronic structure of 4f-atoms adsorbed on metal and Graphene substrates — ●Alexander B. Shick[1], Dmitry S. Shapiro[2], and Alexander I. Lichtenstein[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]nstitute of Radio Engineering and Electronics, Russian Academy of Sciences, Moscow — [3]Institute of Theoretical Physics, University of Hamburg, Germany

Surface supported single magnetic atoms, the so-called "single-atom magnets", open new opportunities in a quest for the ultimate size limit of magnetic information storage. Initially, the research mainly focused on 3d-atoms on surfaces. Recently, the attention was turned to the 4f-atoms, culminating in the experimental discovery of magnetically stable Ho atom on MgO(001) substrate [1], and Dy atom on graphene/Ir(111)[2]. We address the electronic and magnetic character of 4f-atoms on metal and Graphene substrate making use of a combination of the DFT with the exact diagonalization of Anderson impurity model (DFT+ED) [3]. The spin and orbital magnetic moments of Dy@Ir(111) and Dy/Graphene/Ir(111) are evaluated and compared with experimental XMCD data. The magnetic anisotropy energy is estimated, and the magnetic stability is discussed. The role of 5d-4f interorbital exchange polarization in modification of the 4f-shell energy spectrum is emphasized. [1] F. Donati et al., Science 352, 318 (2016). [2] R. Baltic et al., Nano Lett. 16, 7610 (2016). [3] A. B. Shick, D. S. Shapiro, J. Kolorenc, A. I. Lichtenstein, Sci. Rep. 7, 2751 (2017).

DS 38.5   Fri 11:30   HL 001

Interlayer trions in the MoS_2/WS_2 van der Waals heterostructure — ●Thorsten Deilmann and Kristian Sommer Thygesen — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Electronic excitations in van der Waals heterostructures can have interlayer or intralayer character depending on the spatial localisation of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally. In contrast, studies of charged trions have so far been limited to the intralayer type.

Here we investigate the complete set of interlayer excitations in a MoS_2/WS_2 heterostructure using a novel ab-initio method, which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of $18/28$ meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers.

DS 38.6   Fri 11:45   HL 001

The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining — ●Miguel Marques[1] and Antonio Sanna[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Microstrukture Physics, Weinberg 2, 06120 Halle, Germany

Starting from the experimental data contained in the inorganic crystal structure database, we use a statistical analysis to determine the likelihood that a chemical element A can be replaced by another B in a given structure. This information can be used to construct a matrix where each entry (A,B) is a measure of this likelihood. By ordering the rows and columns of this matrix in order to reduce its bandwidth, we construct a one-dimension ordering of the chemical elements, analogous to the famous Pettifor scale. The new scale shows large similarities with the one of Pettifor, but also striking differences,

especially in what comes to the ordering of the non-metals.

DS 38.7 Fri 12:00 HL 001

Novel two-dimensional topological insulators from first principles materials screening — •Thomas Olsen and Kristian Thygesen — Technical University of Denmark

We have applied first principles calculations to find new stable two-dimensional materials with non-trivial band topology. The novel materials include more than 10 quantum spin Hall insulators, quantum anomalous Hall insulators and topological crystalline insulators protected by mirror symmetry. We also discuss the dual topological nature of the band structure in the presence of both time-reversal and mirror symmetry and show that odd mirror Chern numbers always imply a quantum spin Hall effect.

DS 38.8 Fri 12:15 HL 001

Nanoparticles Classification with Self-Organisation Map (SOM) on 3D Electrostatic Potential Surface (EPS) — •Baichuan Sun and Amanda Barnard — Molecular & Materials Modelling, Data61 CSIRO, Door 34 Goods Shed, Village St, Docklands, VIC 3008, Australia

State-of-the-art deep learning (DL) algorithms are having tremendous impact across all scientific fields, and Material Science (MS) is no exception. A combination of computational chemistry simulations and DL techniques requires a hybrid computation/data research workflow, which represents a revolutionary approach to MS studies. There is a gap between the ab initio characterisation of nanomaterials with electronic structure simulations and its analytics with DL frameworks which stems from difficulties in representing quantum mechanical properties in such a way that is suitable for artificial neural networks. To overcome this issue we are evaluating the efficiency of visualising the 3-D Electrostatic Potential Surface (EPS) with Self-organising

Maps (SOM), and integrating them directly into reliable DL frameworks. A Self-organisation Map classifies high-dimensional data into low-dimensional (normally 2D) space without supervision, while retaining the intrinsic topological relationship of the data set. As we will show, it is possible to represent a 3D molecular EPS with a single 2D snapshot, or "fingerprint" of the particle, provided they are orientationally invariant. In this study we demonstrate how Ag nanoparticles 3-D EPS self-organising texture maps can be used to classify nanoparticles based on the energy of the Fermi level.

DS 38.9 Fri 12:30 HL 001

Regulation of structure and high thermoelectric performance of 1D SnTe via encapsulation within single-walled carbon nanotube — Andrij Vasylenko[1], •Jamie Wynn[2], Sam Marks[1], Paulo V. C. Medeiros[3], Quentin M. Ramasse[4], Andrew J. Morris[4], Jeremy Sloan[1], and David Quigley[1] — [1]University of Warwick, Coventry, UK — [2]University of Cambridge, Cambridge, UK — [3]Daresbury Campus, Darsbury, UK — [4]University of Birmingham, Birmingham, UK

We present the extreme case of nanostructuring, exploiting capillarity of single-walled carbon nanotubes (SWCNTs) for synthesis of the smallest possible thermoelectric SnTe nanowires with cross sections as small as a single atom. By adapting high-throughput ab initio random structure searching, we discover several structures of SnTe that can be formed within SWCNT and compare results with experimentally obtained encapsulated SnTe nanowires. From first principles, we demonstrate that by choosing the appropriate diameter of a template SWCNT, we can manipulate the structure of 1D SnTe and its thermoelectric performance. The demonstrated technique opens a practical route towards nanostructural manipulation of electrical and thermoelectric properties of the 1D materials. The best candidate 1D SnTe structures demonstrate strongly enhanced ZT over a unprecedentedly broad temperature range with a maximum value of 3.25.