DS 8: 2D materials (joint session HL/DS)

Time: Monday 15:00–16:30 Location: EW 201

DS 8.1 Mon 15:00 EW 201

Predicting and Understanding Quantum Spin Hall Insulators with the Help of Compressed Sensing/SISSO — Carlos Mera Acosta[1,2], Runhai Ouyang[1], Adalberto Fazzio[2], Matthias Scheffler[1], Luca Ghiringhelli[1], and •Christian Carbogno[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]University of São Paulo, São Paulo, Brazil

Quantum Spin Hall insulators (QSHIs), i.e., two-dimensional insulators with conducting edge states protected by time-reversal symmetry, have attracted considerable scientific interest in recent years. In this work, we perform first-principles calculations to compute the Z_2-invariant for 220 functionalized honeycomb-lattice materials. Using the recently developed sure independence screening and sparsifying operator (SISSO) method [1], we derive a “map of materials”, in which metals, trivial insulators, and QSHIs are spatially separated. The axes of this map are defined by physically meaningful descriptors, i.e., non-linear functions that only depend on the properties of the material’s constituent free atoms. First, this yields fundamental insights into the mechanisms driving topological transitions. Second, we are able to predict the topological character of materials that are not part of the originally investigated set just from their position on the map (predictive power greater than 95%). By this means, we are able to predict 89 yet unknown QSHIs.

[1] Runhai Ouyang *et al.*, *arXiv:1710.03319* (2017).

DS 8.2 Mon 15:15 EW 201

Superconductivity and electron-phonon properties of intrinsic and doped antimonene — •Andrei Lugovskoi, Mikhail Katsnelson, and Alexander Rudenko — Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen, The Netherlands

Antimonene is a recently discovered elemental 2D phase of Sb with buckled honeycomb structures. The material was successfully obtained experimentally, and posses interesting set of properties. It was shown to have high stability on base of both experimental observations and *ab initio* modeling, and is also predicted to have interesting optical properties and strain tunable band gap. At the same time, superconductivity in doped phosphorene and graphene was recently observed experimentally, which opens new opportunities for the application of 2D materials.

We present the *ab initio* calculations of electron-phonon coupling properties and critical superconducting temperature in both n- and p-doped antimonene at experimentally achievable carrier concentrations. The effects of small strains and bias voltage on the critical temperature are also considered. Required quantities are obtained by using density functional theory implementation of electron-phonon Wannier-Fourier interpolation in EPW and QE codes. Critical temperature at various carrier densities is estimated using McMillan-Allen-Dynes equation.

The work is a part of the research program "Two-dimensional semiconductor crystals" (prj. 14TWOD01), which is partly financed by the Netherlands Organization for Scientific Research (NWO).

DS 8.3 Mon 15:30 EW 201

Dielectric Engineering of Intra-excitonic Correlations in a van der Waals Heterostructure — •Philipp Steinleitner[1], Philipp Merkl[1], Alexander Graf[1], Philipp Nagler[1], Christian Schüller[1], Tobias Korn[1], Rupert Huber[1], Samuel Brem[2], Malte Selig[3], Gunnar Berghäuser[2], and Ermin Malic[2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — [3]Department of Theoretical Physics, Technical University of Berlin, Berlin, Germany

Atomically thin transition metal dichalcogenide monolayers promise novel optoelectronic applications due to their direct bandgap in the optical range. Reduced Coulomb screening, in combination with the two-dimensionality, stabilizes excitons, even at room temperature. Due to the extreme confinement perpendicular to the plane of the material, excitons are particularly sensitive to the local surrounding environment. Thus, capping the monolayer with a dielectric material allows one to non-invasively change their hydrogen-like structure. Here we report how an insulating hexagonal boron nitride cover layer influences the intra-excitonic 1s-2p transition. Using time resolved pump/THz probe techniques, we trace both optically bright and dark exciton states and are able to extract quantitative information about transition energies and linewidths. We find that the cover layer redshifts the 1s-2p transition and leads to a decrease of its linewidth. Using microscopic modelling, we show that our experimental data also support the formation of dark excitons from an initially bright population.

DS 8.4 Mon 15:45 EW 201

high-throughput search of novel 2d materials for electronic and optoelectronic applications — •davide campi, thibault sohier, antimo marrazzo, marco gibertini, nicolas mounet, and nicola marzari — Theory and simulation of materials (THEOS) and national center for computational design and discovery of novel materials (MARVEL), école polytechnique fédéral lausanne, ch-1015, lausanne, switzerland

2D materials provide a novel paradigm and toolbox for materials scientists to discover or engineer new properties and functionalities. However, the handful of 2D materials intensively studied up to now represent only a few of the manifold possibilities. In this work we present the results of an applications-oriented screening that, using state-of-the-art first-principles simulations and automatized high-throughput calculations through the AiiDA platoform[1], identifies new promising candidates for field effect transistors (FET), photocatalytic water splitting and nanoporous crystalline membranes, selected among the hindreds of 2D materials (1844)[2] discovered by performing a ”computational exfoliation” of a dataset of more than 100000 bulk parent structures.

[1] G.Pizzi, A.Cepellotti, R.Sabatini, N.Marzari and B.Kozinsky, Comp. Mat. Sci. 111, 218 (2016). [2] N.Mounet, M.Gibertini, P.Schwaller, D.Campi, A.Merkys, A.Marrazzo, T.Sohier, I.E.Castelli, A.Cepellotti, G.Pizzi and N.Marzari, in press (2018).

DS 8.5 Mon 16:00 EW 201

Spin- and valley-dependent transport through a 2D semiconductor with magnetic substrate — •Gerhard Fechteler, Andor Kormányos, and Guido Burkard — University of Konstanz, Germany

Motivated by recent theoretical [1] and experimental [2,3] works, we study spin- and valley-dependent electron scattering in monolayers of transition metal dichalcogenides through a region with an underlying magnetic substrate. The valley splitting and changes in the parameters such as Fermi velocity and effective electron mass induced by the magnetic substrate lead to novel spin- and valley selection possibilities compared to gated structures [4]. Neglecting Rashba spin-orbit coupling (SOC), we study the Fermi energy and incident angle dependence of spin and valley selective scattering processes. Moreover, we find pronounced and tuneable Goos-Hänchen shifts. In the presence of Rashba SOC, we find that the transmitted and reflected electron beams are split due to spin mixing in the scattering region. Such a spin-dependent scattering can prove useful for the design of novel spintronic devices. [1] J. Qi et al., Phys. Rev. B 92, 121403 (2015). [2] C. Zhao et al., Nat. Nanotechnol. 12, 757-760 (2017). [3] D. Zhong et al., Sci. Adv. 3, e1603113 (2017). [4] H. Ghadiri et al., J. Phys.: Condens. Matter 29, 115303 (2017).

DS 8.6 Mon 16:15 EW 201

Electron quantum optics in anisotropic pseudospin one systems — •Yonatan Betancur Ocampo and Dario Bercioux — Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 4 20018 Donostia-San Sebastián, Spain

We proposed the development of electron quantum optics devices through heterojunctions formed by anisotropic and relativistic pseudospin one materials. Based on our theoretical calculations, we found that the probability transmission, reflection and refraction law present atypical behavior. We have shown that collimation effect, Veselago lenses, and beam splitters are enhanced using pseudospin one particles. Moreover, novel quantum optics devices could be designed such as asymmetric Veselago and diverging lenses. Our findings suggest that these devices can be built from the strain-engineering of Lieb lattices.