O 72: 2D Materials 3: hBN and Electronic Structure

Time: Thursday 15:00–17:00 Location: S052

O 72.1 Thu 15:00 S052

Electronic Structure of Two-Dimensional CoO2 — Ann Julie U. Holt[1], Sahar Pakdel[1], Jonathan Rodríguez-Fernández[2], Yu Zhang[3], Davide Curcio[1], Zhaozong Sun[4], Paolo Lacovig[5], Yong-Xin Yao[6,7], Jeppe V. Lauritsen[4], Silvano Lizzit[5], Nicola Lanatà[1,8], Philip Hofmann[1], Marco Bianchi[1], and •Charlotte E. Sanders[3] — [1]Dept. of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus Univ., 8000 Aarhus, DK — [2]Dept. of Physics, Univ. of Oviedo, Oviedo 33007 ES — [3]UK Central Laser Facility, RCaH, STFC RAL, Didcot, Oxfordshire OX11 0QX, UK — [4]Interdisciplinary Nanoscience Center (iNANO), Aarhus Univ., 8000 Aarhus, DK — [5]Elettra Sincrotrone Trieste S.C.p.A., AREA Science Park, Strada Statale 14, km 163.5, 34149 Trieste, IT — [6]Ames Laboratory U.S.-DOE, Ames, IA 50011, USA — [7]Dept. of Physics and Astronomy, Iowa State Univ., Ames, IA 50011, USA — [8]Nordita, KTH Royal Institute of Technology and Stockholm Univ., Roslagstullsbacken 23, 10691 Stockholm, SE

The transition metal oxide CoO2 forms bulk layered structures that exhibit complex correlated electronic states. However, little has been known about the electronic properties of the isolated single layer. We have now [1] studied CoO2/Au(111), using angle-resolved photoemission spectroscopy, x-ray photoelectron diffraction, and density functional theory. The results of our study show single-layer CoO2 to be metallic, with electronic correlations. They emphasize the interest of oxides as a new subject within two-dimensional materials research. [1] 2D Mater. 8 (2021) 035050.

O 72.2 Thu 15:15 S052

Unified Treatment of Magnons and Excitons in Monolayer CrI3 from Many-Body Perturbation Theory — •Thomas Olsen — Technical University of Denmark

We present first principles calculations of the two-particle excitation spectrum of CrI3 using many-body perturbation theory including spin-orbit coupling. Specifically, we solve the Bethe-Salpeter equation, which is equivalent to summing up all ladder diagrams with static screening, and it is shown that excitons as well as magnons can be extracted seamlessly from the calculations. The resulting optical absorption spectrum as well as the magnon dispersion agree very well with recent measurements, and we extract the amplitude for optical excitation of magnons resulting from spin-orbit interactions. Importantly, the results do not rely on any assumptions of the microscopic magnetic interactions such as Dzyaloshinskii-Moriya (DM), Kitaev, or biquadratic interactions, and we obtain a model independent estimate of the gap between acoustic and optical magnons of 0.3 meV. In addition, we resolve the magnon wave function in terms of band transitions and show that the magnon carries a spin that is significantly smaller than $\hbar$. This highlights the importance of terms that do not commute with S_z in any Heisenberg model description.

[1] T. Olsen, Phys. Rev. Lett. 127, 166402, (2021)

O 72.3 Thu 15:30 S052

Excitons in two-dimensional magnetic semiconductors — •Marie-Christin Heissenbüttel, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Semiconducting two-dimensional magnets exhibit peculiar interrelation between magnetic properties and light-matter interaction. We will present and discuss ab-initio GW/Bethe-Salpeter equation calculations to examine excitonic states in different magnetic systems.
Due to the hexagonal crystal structure the out-of-plane ferromagnetic monolayer CrI_3 came to the fore for the construction of heterobilayers with transition-metal dichalcogenides [1]. Due to coupling effects the magnetic properties are transferred and can be observed in a splitting and a modified Zeeman effect of the excitons. On the other hand, CrSBr shows in-plane magnetization in combination with a large crystal anisotropy. This is reflected in the quasi-1D behavior of different opto-electronic properties [2].
[1] Nano Lett. Lett. 21, 5173-5178 (2021)
[2] https://arxiv.org/abs/2205.13456

O 72.4 Thu 15:45 S052

Nanoscale view of massive Dirac quasiparticles in lithographic superstructures — •Alfred Jones[1], Lene Gammelgaard[2], Deepnaryan Biswas[1], Mikkel Sauer[3], Roland Koch[4], Chris Jozwiak[4], Eli Rotenberg[4], Aaron Bostwick[4], Kenji Watanabe[5], Takashi Taniguchi[5], Cory Dean[6], Thomas Pedersen[3], Antti-Pekka Jauho[2], Peter Bøggild[2], Bjarke Jessen[6], and Søren Ulstrup[1] — [1]Aarhus University, Denmark — [2]Technical University of Denmark, Denmark — [3]Aalborg University, Denmark — [4]Advanced Light Source, USA — [5]National Institute for Materials Science, Japan — [6]Columbia University, USA

Massive Dirac quasiparticles play a central role in a number of emerging physical phenomena such as topological phase transitions and anomalous Hall effects. Single-layer graphene appears to be an ideal platform to explore such properties, however engineering the transition from massless to massive Dirac quasiparticles in a controllable fashion remains a significant challenge. Here, we employ angle-resolved photoemission with a nanoscale light spot (nanoARPES) to directly measure the electronic structure modifications induced by lithographic patterning of an antidot superlattice onto a graphene device. We observe a transition from massless Dirac fermions in the pristine graphene to a massive character in patterned regions, and determine that the mass scales linearly with antidot diameter, consistent with theory. Gate-induced electron-doping of the patterned graphene produces an enhancement of the mass, highlighting the versatility of nanopatterned graphene as a platform for engineering such quasiparticles.

O 72.5 Thu 16:00 S052

Tuning lower dimensional superconductivity with hybridization at a superconducting-semiconducting interface — •Anand Kamlapure[1], Manuel Simonato[1], Emil Sierda[1], Manuel Steinbrecher[1], Umut Kamber[1], Elze J. Knol[1], Peter Krogstrup[2], Mikhail I. Katsnelson[1], Malte Rösner[1], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, the Netherlands — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark

Study of influence of interface electronic structure on the superconductivity (SC) in lower dimensions is important to tune SC in view of its applications to gated superconducting electronics, and superconducting layered heterostructures. Here, using ultra-low temperature scanning tunneling microscopy and spectroscopy, we demonstrate the formation of hybrid electronic structure at the interface between a lead film and black phosphorus. We show that interfacial hybridization weakly modifies the confinement potential and leads to a renormalization of the superconducting gap and a strong modification of the observed vortex structure. Using ab initio methods combined with analytical modeling, we link the renormalized gap to a weighting of the superconducting order parameter in reciprocal space. These results illustrate that interfacial hybridization can be used to tune SC in quantum technologies based on lower dimensional superconducting electronics. Reference: arXiv:2109.08498 (2021).

O 72.6 Thu 16:15 S052

Diversity of defect-related excitons in hBN from ab initio calculations — •Alexander Kirchhoff, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Westfälische Wilhelms-Universität Münster, Institut für Festkörpertheorie, Wilhelm-Klemm-Straße 10, 48149 Münster

While pristine hexagonal boron nitride (hBN) is an insulator with an optical gap of ∼5 eV, point defects in this material are discussed as single-photon emitters in the visible optical spectrum. In this study, we examine different defects consisting of carbon or oxygen substitutions and vacancies in an hBN monolayer from an ab initio approach, via the GW/BSE approximation. Our results show deep defect states and defect-related excitations with energies in the visible regime. We present a detailed analysis of their structure and energetic composition and furthermore discuss the dependence of the excitonic spectrum on the geometry. Finally, we present a defect of two carbon substitutions adjacent to a divacancy, which shows an antiferromagnetic ground state.

O 72.7 Thu 16:30 S052

Engineering magnetic interactions in magnetic thin films

with two-dimensional materials — •Hangyu Zhou[1,2], Manuel dos Santos Dias[1,3,4], Weisheng Zhao[2], and Samir Lounis[1,3] — [1]Peter Grünberg Institut and Institute for Advanced Simulations, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]School of Integrated Circuit Science and Engineering, MIIT Key Laboratory of Spintronics, Beihang University, Beijing 100191, China — [3]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — [4]Scientific Computing Department, STFC Daresbury Laboratory, Warrington WA4 4AD, United Kingdom

Two-dimensional (2D) materials have received great attention due to their unique physical and chemical properties and ease of integration in heterostructures, which can lead to improved magnetic properties. Here, we explore with density functional theory calculations the impact of monolayers of graphene and hexagonal boron nitride (h-BN) on the magnetism and structural properties of a Co monolayer placed on Pt(111) and Au(111) surfaces. In particular, we investigate how the magnetic interactions, such as the Heisenberg exchange interaction and the Dzyaloshinskii-Moriya interaction (DMI), are influenced by the 2D monolayer and by structural reconstructions, which in turn can be utilized to ignite complex spin-textures. These results may contribute to an enhanced tunability of skyrmion formation in such composite magnetic heterostructures.

O 72.8 Thu 16:45 S052

Threshold Energies for Defect Production in 2D Materials under Low Energy Ion bombardment: Insights from ab-initio Molecular Dynamics — •Silvan Kretschmer, Sadegh Ghaderzadeh, Stefan Facsko, and Arkady V. Krasheninnikov — Helmholtz-Zentrum Dresden-Rossendorf, Germany

Low energy ion implantation (LEII) provides a valuable tool to tune the mechanical, electronic and catalytic properties of 2D materials by the targeted implantation of impurities. In contrast to ion irradiation at higher energies the commonly applied binary collision formula fails to describe the outcome of the irradiation process for ions close to the displacement energy, that is the minimum ion energy needed to displace the target atom. The dominating influence of the chemical interaction of projectile and target atoms and its effect on the displacement energy are adressed in this work. For that, we carried out ab-initio molecular dynamics (MD) simulations for a broad range of projectiles (elements Hydrogen to Argon) impacting on graphene and h-BN, and determined the energies needed to displace C, N and B atoms, respectively. We further present and validate a scheme to incorporate the effect of spin-polarization on the displacement process - as spin-polarized ab-initio MD runs tend to fail at bond-breaking.