O 22: 2D Materials II: Electronic Structure (joint session O/TT)

Time: Tuesday 10:30–12:15 Location: MA 005

O 22.1 Tue 10:30 MA 005

On the origin of circular dichroism from graphene, WSe_2, and other quantum materials — •Lukasz Plucinski — PGI-6 Forschungszentrum Jülich

On the example of graphene, within the dipole approximation, we discuss various contributions to the circular-dichroic angle-resolved photoemission (CD-ARPES) [1] which include phase shifts of the participating partial waves in the atomic photoionization [2], the finite inelastic mean free path induced CD [3], the interatomic phase shifts [4], and the CD due to multiple scattering of the excited electron [5]. Using tabulated phase shifts and radial integrals [6], we predict photon energies at which CD signal might exhibit sign changes, and compare the prediction to experimental results. Subsequently, we perform similar analysis for WSe_2, a material where orbital characters are relatively well-defined, however, varying over Brillouin zone, with different contributions at K, K', and Γ points. This can be translated into understanding CD-ARPES from topological materials. Within this context, we briefly discuss how various components needed to derive the Berry curvature, the spin characters [4], and the phases of the wave functions, can be accessed through CD-ARPES and its spin-polarized variant.

[1] Plucinski, arXiv:2309.02187 (2023), [2] Dubs et al., Phys. Rev. B 32, 8389 (1985) [3] Moser, JESRP 214, 29 (2017) [4] Heider, et al., PRL 130, 146401 (2023) [5] Daimon et al., JJAP 32, L1480 (1993) [6] Goldberg et al., JESRP 21, 285 (1981)

Topical Talk O 22.2 Tue 10:45 MA 005

Bias free extraction of orbital angular momentum from two-dimensional materials by dichroic photoemission — Jonas Erhardt[1,2], Cedric Schmitt[1,2], Philipp Eck[2,3], Philipp Kessler[1,2], Kyungchan Lee[1,2], Giorgio Sangiovanni[2,3], Ralph Claessen[1,2], and •Simon Moser[1,2] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

Topological band inversion is at the heart of the quantum spin Hall insulator (QSHI) but is difficult to demonstrate experimentally. In the bulk, this band inversion is characterized by the Berry curvature, a gauge-invariant fingerprint of the wave function's geometric properties. Intimately tied to orbital angular momentum (OAM), the Berry curvature can be in principle extracted from circular dichroism in angle-resolved photoemission spectroscopy (CD-ARPES), were it not for interfering photoelectron emission channels that obscure the OAM signature. Here, we outline a full-experimental strategy to avoid such interference artifacts and isolate the clean OAM from the CD-ARPES response. Bench-marking this strategy for the recently discovered atomic monolayer QSHI indenene, we establish CD ARPES as scale-able bulk probe to experimentally classify the topology of two dimensional quantum materials with time reversal symmetry.

O 22.3 Tue 11:15 MA 005

Orbital angular momentum of $Cr_2Ge_2Te_6$ bands using circular dichroism — •Honey Boban[1], Mohammed Qahosh[1], Xiao Hou[1], Tom G Saunderson[2,3], Yuriy Mokrousov[2,3], Claus Michael Schneider[1], and Lukasz Plucinski[1] — [1]Peter Gruenburg Institute-6, Forschungszentrum Juelich, Germany — [2]Peter Gruenburg Institute-1, Forschungszentrum Juelich, Germany — [3]University of Mainz, Germany

We present high-resolution circular-dichroic angle-resolved photoemission (CD-ARPES) spectra from graphene, WSe_2, and $Cr_2Ge_2Te_6$ (CGT), materials that exhibit different levels of band structure complexity. In graphene, where bands near the Fermi level are of single C $2p_z$ orbital nature, we investigated various contributions to dichroism, such as phase shifts and final state scattering, by varying the photon energy. In WSe_2, near the valence band maximum Γ and K points we found strong contribution of dichroism derived from the experimental geometry, in the light incidence angle dependent CD-ARPES. We use these findings to study the OAM texture of a 2D ferromagnetic material CGT [1], in which the time reversal symmetry is broken and mirror planes are absent. CGT is interesting as it offers a platform to study the interplay of ferromagnetism and spin orbit coupling, and is a potential candidate for future spintronic devices where both spin degree of freedom and orbital degree of freedom can be utilized. Therefore, understanding the initial band OAM in CGT is crucial, as it is closely linked to its quantum transport properties [2]. Ref: [1] J. Phys. Condens. Matter **7**, 69(1995), [2] Rev. Mod. Phys. **82**, 1539(2010)

O 22.4 Tue 11:30 MA 005

Evolution of band structure in 2D Transition Metal Dichalcogenide alloy $Mo_xW_{1-x}Se_2$ — •Sarath Sasi[1], Laurent Nicolaï[1], Aki Pulkkinen[1], Christine Richter[2,3], Karol Hricovini[2,3], and Ján Minár[1] — [1]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, CY Cergy Paris Université, Neuvillesur- Oise, France — [3]Université Paris-Saclay, CEA, CNRS, LIDYL, Gif-sur-Yvette, France

In the realm of two-dimensional (2D) materials research, transition metal dichalcogenides (TMDCs) have emerged as significant subjects, especially WSe_2 and $MoSe_2$, which are notable for their similar band structures. Our research aims to explore the band structure evolution in $Mo_xW_{1-x}Se_2$ alloys (x= 0 to 1) utilizing a blend of Angle-Resolved Photoemission Spectroscopy (ARPES) experimentally and its complementary theoretical one-step model photoemission calculations employing the *SPR-KKR* package [1]. Furthermore, circular dichroism [2] ARPES measurements provide an insight into the orbital characteristics, revealing Mo concentration-dependent effects that are substantiated through photoemission calculations using the coherent potential approximation(*CPA*). For homogeneous random alloys, *CPA* effectively models average scattering properties and, within the KKR formalism, ensures no extra scattering when embedding an alloy component. Studying these systems with inherent disorders uncovers fundamental insights, enhancing their potential applications.

[1]Braun, J., Minar, J., Ebert, H. (2018). Physics Reports, 740.
[2]Beaulieu, S. *et al* . (2020). Physical Review Letters, 125(21).

O 22.5 Tue 11:45 MA 005

Photon energy dependence of circular dichroism in the topologically nontrivial surface states of WTe_2 — •Aki Pulkkinen[1], Ján Minár[1], Shoresh Soltani[2], Khadiza Ali[2], Craig Polley[2], Balasubramanian Thiagarajan[2], and Saroj Dash[2] — [1]New Technologies-Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]MAX IV Laboratory, Lund University, Lund, Sweden

We present a theoretical and experimental study of the distorted octahedral transition metal dichalcogenide T_d-WTe_2, a type-II Weyl semimetal renowned for its intriguing physical properties, such as strong spin-orbit coupling, giant magnetoresistance, and superconductivity. Utilizing the full potential formulation of the one-step model of photoemission, our investigation focuses on elucidating the electronic and topological properties of WTe_2. By employing the theoretical model of angle-resolved photoemission spectroscopy (ARPES) and circular dichroism (CD), our results provide detailed insights into the spin texture of electronic states near the Fermi level. These findings contribute to the ongoing exploration of WTe_2, emphasizing its potential applications in quantum computing and advanced electronic devices while bridging the gap between theoretical predictions and experimental observations, including the characteristics of surface states.

O 22.6 Tue 12:00 MA 005

Ultrafast Hidden Spin Polarization Dynamics of Bright and Dark Excitons in 2H-WSe2 — •Mauro Fanciulli[1,2], David Bresteau[2], Jérome Gaudin[3], Shuo Dong[4], Romain Géneaux[2], Thierry Ruchon[2], Olivier Tcherbakoff[2], Jan Minar[5], Olivier Heckmann[1,2], Maria Christine Richter[1,2], Karol Hricovini[1,2], and Samuel Beaulieu[3] — [1]LPMS, CY Cergy Paris Université, 95031 France — [2]Université Paris-Saclay, CEA, CNRS, LIDYL, 91191 France — [3]Université de Bordeaux - CNRS - CEA, CELIA, 33405 France — [4]Beijing National Laboratory for Condensed Matter Physics, 100190 China — [5]University of West Bohemia, 30100 Czech Republic

We performed spin-, time- and angle-resolved extreme ultraviolet photoemission spectroscopy of excitons prepared by photoexcitation of inversion-symmetric 2H-WSe2 with circularly polarized light.

The very short probing depth of XUV photoemission permits selective measurement of photoelectrons originating from the top-most WSe2 layer, allowing for direct measurement of hidden spin polariza-

tion of bright and momentum-forbidden dark excitons.

Our results reveal efficient chiroptical control of bright excitons' hidden spin polarization. Following optical photoexcitation, intervalley scattering between nonequivalent K-K' valleys leads to a decay of bright excitons' hidden spin polarization. Conversely, the ultrafast formation of momentum-forbidden dark excitons acts as a local spin polarization reservoir, which could be used for spin injection in van der Waals heterostructures involving multilayer transition metal dichalcogenides.