DS 50: Optics and Light-Matter Interaction with Excitons in 2D Materials (Joint Session HL, DS, O, and TT, organized by DS)

Time: Friday 11:15–12:15 Location: CHE 89

DS 50.1 Fri 11:15 CHE 89

Enhanced light-matter interaction in graphene/h-BN van der Waals heterostructures — •Caterina Cocchi[1], Wahib Aggoune[1,2], Dmitrii Nabok[1], Karim Rezouali[2], Mohamed Akli Belkhir[2], and Claudia Draxl[1,2] — [1]Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Laboratoire de Physique Théorique, Faculté des sciences exactes, Université de Bejaia, 06000 Bejaia, Algeria

Investigating the electronic and optical properties of graphene/h-BN heterostructures from first principles, we observe a peculiar nature of their excitations. To this extent, we employ density-functional and many-body perturbation theory in terms of the GW approximation and the Bethe-Salpeter equation. The interaction with h-BN opens a gap in graphene, making the heterostructures semiconducting. These systems absorb light over a broad frequency range, from the near-infrared to the ultraviolet region, exhibiting novel features induced by the stacking. While the specific properties of the building blocks are basically preserved, the inter-layer electron-hole pairs that are formed in the heterostructure can be modulated upon layer patterning. By choosing the stacking arrangement, the electronic coupling between the individual components can be tuned to enhance light-matter interaction. Our results open up perspectives in view of designing new low-dimensional materials with tailored opto-electronic characteristics.

DS 50.2 Fri 11:30 CHE 89

Spectral Focusing of Broadband Silver Electroluminescence in Nanoscopic FRET-LEDs — •Robin Puchert, Florian Steiner, Gerd Plechinger, Felix Hofmann, Christian Schüller, Tobias Korn, Jan Vogelsang, Sebastian Bange, and John Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstrasse 31, 93053 Regensburg, Germany

A challenge in LED technology is the use of fluorescence resonance energy transfer (FRET) in spectral conversion. An LED based on FRET effect would show both up- and down-conversion of electroluminescence (EL), since the electrically driven resonance of the light emitting device (donor) couples non-radiatively to the acceptor fluorophore resonance.

FRET-LEDs have already been proposed. However, such devices have yet to be demonstrated. The challenge lies in generating light electrically in close proximity to a dipolar acceptor in order to allow near-field coupling. We present a solution to this problem by combining a lateral LED structure with a two-dimensional transition-metal dichalcogenide overlayer (TMDC). The LED's entire excitation energy is transferred to the 2D crystal overlayer through resonant dipole-dipole coupling rather than by trivial reabsorption. This is quite remarkable given the fact that such an atomically thin TMDC monolayer absorbs only a mere 4 % of light. By using plasmonic silver nanoparticle junctions to generate broad-band EL coming from sub-diffraction localized hotspots, we see dramatic spectral focusing of the EL into the narrow excitonic resonance of the atomically thin overlayer.

DS 50.3 Fri 11:45 CHE 89

Spin-flip transitions induced by time-dependent electric fields in tuned Transition Metal Dichalcogenides magnetic thin films. — •Omar Messaoudi[1,2], Julen Ibañez-Azpiroz[2], Hamid Bouzar[1], and Samir Lounis[2] — [1]Université Mouloud Mammeri de Tizi Ouzou, Tizi Ouzou, Algeria — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

We study from first principles the relativistic electron structure of Transition Metal Dichalcogenides such as MoS_2 and WS_2 on top of which Iron is deposited as a monolayer or as a single impurity. The resulting systems turn out to be magnetic and, in particular, the states near the Fermi level show a non-negligible noncollinear spin-polarization due to the effect of spin-orbit coupling. In these noncollinear states, we analyze the excitations induced by a time-dependent electric field employing a formalism based on the maximally localized Wannier functions [1]. Finally, we analyze the absorption spectrum of circularly polarized light and discuss the possibility of observing a dichroic signal.

[1] J. Ibañez-Azpiroz *et. al*, Phys. Rev. Lett. **109**, 156401 (2012)

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DS 50.4 Fri 12:00 CHE 89

Ab-initio calculations of valley depolarization in single-layer WSe_2 mediated by electron-phonon interaction — Alejandro Molina-Sánchez[1], Davide Sangalli[2], Andrea Marini[2], and •Ludger Wirtz[1] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Istituto de Strutura della Materia (CNR), CNR, Monterrotondo, Rome, Italy

Circularly polarized light can be used to selectively populate the K^+ and K^- electronic valleys of single-layer WSe_2. Valley depolarization has been measured through time-dependent Kerr experiments (measuring the rotation of a linearly polarized probe pulse applied after a circularly polarized pump pulse) by several groups. However, the depolarization mechanism still remains largely debated. Using an ab-initio implementation of time-dependent many-body perturbation theory (including electron-electron, electron-hole, and electron-phonon interaction), we solve unambiguously the debate about the dominant mechanism that drives the valley depolarization. The decay dynamics and peculiar temperature dependence (observed in recent experiments) is explained in terms of electron-phonon mediated processes that induce spin-flip inter-valley transitions.