UNIVERSITÄT DUISBURG ESSEN

PHYSIK E=

Physikalisches Kolloquium

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13:00 Uhr
MC 122

Ultrafast charge dynamics and optical response in 2D materials: interplay of excitons and phonons

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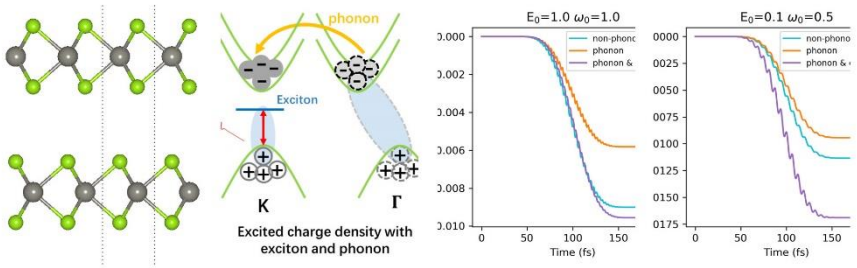

The last decade has seen a concerted effort in accelerating the discovery of materials for energy needs, which has facilitated close collaboration between experiment and theory. In this talk, I will focus on some intriguing chemical and optical properties of 2D materials that have so emerged. I will show that defects in 2D materials, such as the versatile insulator h-BN or the lubricant MoS2, may tune their electronic structure turning them into promising catalyst for hydrogenation of CO21 or CO2 into methanol. On the other hand, the large exciton binding energy together with strong interactions between electrons, excitons, and phonons, show potential for application of these 2D materials in energy harvesting. I will show, through application of time dependent density functional theory and many-body theory, that the (momentum-resolved) intra- and inter-valley charge dynamics, and photoluminescence in these 2D materials is a result of a complex collective response involving free electrons/holes, bright and dark excitons, and phonons.3 I will make contact with available experimental data, and hope to convince you that advances in ab initio calculations are now poised to help design novel 2D materials for a sustainable future.

1. K. Chagoya, et al., ACS Sustainable Chemistry & Engineering 9, 2447 (2021).
2. D. Le, et al., J. Chem. Phys. 154, 174701 (2021).
3. J. Shi, V. Turkowski, and T. S. Rahman, Phys. Rev B 107, 155431 (2023).