MM 10: Materials for Storage and Conversion of Energy: New Storage Materials

Time: Monday 15:45–16:45 Location: SCH A 215

MM 10.1 Mon 15:45 SCH A 215

Improving the cleanliness of TEM investigation of catalyst samples — •Julia Menten[1], Robert Schlögl[1,2], and Walid Hetaba[1] — [1]Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany — [2]Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Transmission electron microscopy (TEM) offers a powerful tool for the analysis of specimens down to an atomic scale. In order to achieve high quality data, sample preparation is a crucial step. Many samples contain a high carbon content, e.g. as organic ligands or solvents. Electron beam exposure can lead to the deposition of carbon on the specimen surface and limit the image resolution and quality of obtained spectroscopic data. Different mitigation strategies can be applied in order to reduce contamination, though these methods can easily harm the specimens or lead to accumulation of carbonaceous molecules in the microscope environment [1].

In our work we focus on the removal of undesirable carbon species before the sample is inserted into the microscope. Our sample cleaning setup allows to investigate the influence of different preparation parameters, e.g. drying time or temperature, on how long solvents remain in the vacuum system and therefore can have an impact on the TEM analysis. Evaluation of the decrease in pressure while pumping our setup with a TEM sample gives insight in necessary drying times. The impact of our sample treatment can be investigated in the TEM by evaluating contrast and thickness measurements.

[1] Mitchell, Micron 73 (2015) 36-46

MM 10.2 Mon 16:00 SCH A 215

Ultrafast Electron Transfer in Photoexcited Fullerene-Derivatives — •Mohamed E. Madjet, Adrian Dominguez-Castro, Fulu Zheng, and Thomas Frauenheim — Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany

Fullerene derivatives continue to attract a lot of interest both experimentally and theoretically. They have been known to be excellent electron acceptors due to their interesting ground and excited state properties. The chemical functionalization of fullerenes makes possible to synthesize and develop new compounds. These derivatives are used as building blocks for molecular complexes and devices with potential applications in solar cells, sensing and in biomedical applications. Using non-adiabatic molecular dynamics simulations combined with time-dependent density functional theory [1-3], we study the photoinduced electron dynamics and charge transfer processes in some fullerene derivatives upon a selective and localized excitation on the donor molecule. Results on hot electron dynamics, charge transfer and nonradiative recombination processes will be presented, discussed, and compared to the experimental results in [4].

References

[1] Madjet et al, PRL 126, 183002(2021) [2] Smith, Shakiba and Akimov, J.Chem. Theory Comp. 17, 678 (2021). [3] Shakiba, Stippel and Akimov, J. Chem. Theory Comp., in print (2022) [4] Julio R. Pinzo et al, J. Am. Chem. Soc. 131, 7727 (2009)

MM 10.3 Mon 16:15 SCH A 215

Carrier Multiplication in Transition Metal Dichalcogenides Beyond Threshold Limit — •Yuxiang Liu[1], Thomas Frauenheim[1], and ChiYung Yam[2] — [1]Bremen Center for Computational Materials Science, University of Bremen, Am Fallturm 1, 28359 Bremen, Germany — [2]Shenzhen Institute for Advanced Study, University of Electronic Science and Technology of China, Shenzhen, 518000, China

Carrier multiplication (CM), multiexciton generation by absorbing a single photon. Beard et al. predicted that CM could overcome the Schokley-Queisser limit and raise solar cell efficiency to ~46%[1]. The current state-of-the-art nanomaterials including quantum dots and carbon nanotubes have demonstrated CM phenomenon, but not satisfactory owing to high threshold energy and inherent difficulties with carrier extraction. We found a below threshold limit CM in monolayer transition metal dichalcogenides (TMDCs) MX2 (M = Mo, W; X= S, Se, Te). Surprisingly, the threshold energy of CM in monolayer TMDCs can be substantially reduced due to lattice vibrations. Electron-phonon couplings (EPC) could cause significant changes in electronic structures, even trigger semiconductor-metal transition, and eventually decrease the threshold energy of CM to less than twice bandgap[2]. Our results identify TMDCs as attractive candidate materials for efficient optoelectronic devices with the advantages of high photoconductivity and phonon-assisted tunable CM characteristics.

Reference [1] Beard, M. C., et al., Acc. Chem. Res.,46, 1252–1260(2013). [2] Yuxiang L., et al., Adv. Sci., 9, 2203400 (2022).

MM 10.4 Mon 16:30 SCH A 215

Vibronic quantum coherences in orthorhombic lead halide perovskite — •Ajay Jha[1,2], Zihui Liu[5], Vandana Tiwari[2], Pabitra Nayak[3], Henry Snaith[3], Xian-Ting Liang[5], R. J. Dwayne Miller[4], and Hong-Guang Duan[5] — [1]Rosalind Franklin Institute, Didcot, UK — [2]MPI-Structure and Dynamics of Matter, Hamburg, Germany — [3]University of Oxford, Oxford, UK — [4]University of Toronto, Toronto, Canada — [5]Ningbo University, Ningbo, China

To unravel the quantum coherent dynamics in orthorhombic perovskite, we employ the ultrafast two-dimensional coherent spectroscopy in methylammonium lead iodide perovskite at 15 K. The data clearly resolve the exciton and carrier band in perovskite along with the interaction between exciton and carriers by observation of cross peaks. The ultrafast population transfer from charge carriers to exciton in perovskite is associated with the vibrational coherences. The nature and role of these coherences will be discussed in detail.