Seminar announcement

Monday, July 14, 2025
10:00 am
WSI, Seminar room S 101

Exclusively in person

Julian is visiting TUM from July 14-16. Please contact David (david.egger@tum.de) in case you would like to meet with him.

"On the metastability of CsPbI3 Perovskite and how to tame it"

A new generation of semiconducting materials based on metal halide perovskites has been launched into the scientific spotlight, exhibiting outstanding optoelectronic properties and providing promise for the development of efficient optical devices. As a vivid example, solar cells made from these materials have quickly reached conversion efficiencies on par with well-established technologies, like silicon. Their widespread success is due, in part, to a unique ability to retain high-quality optoelectronic performance while being easily solution-processed into thin films. However, the interesting photophysics of metal halide perovskites come with a catch; their soft ionic structure promotes complex thermal-induced phase transitions and a variety of dynamic structural behaviours. Such properties have ultimately made understanding several important structure–property relationships ambiguous and obstructed a clear technological path due to inherent structural instability.

This seminar aims to highlight the fundamental aspects of metal halide perovskites that dictate a stable crystal structure, through the lens of thermodynamic preference and phase formation energies. Taking the all-inorganic CsPbI3 system as a suitable case study, we focus on several ways in which its thermodynamically unstable perovskite structure can be maintained at room temperature and elucidate the restructuring pathways taken during destabilization. In addition, we will discuss the origin and mechanisms of phase decay within real-world devices, with emphasis made toward direct visualization using advanced in situ techniques and arriving at quantitative results. For several notable features of halide perovskites dealt with in this contribution, e.g., strain and compositional stabilization, environmental phase triggers, nonperovskite phase restructuring pathway, and lattice anchoring, we attempt to rationalize them using state-of-the-art materials modelling techniques.

It is within this spirit that we not only modify a broad range of properties existing within metal halide perovskites, but regulate them for enhanced functionality. We anticipate that providing a clear perspective for these topics will help deepen our knowledge of the nature of ionic semiconductors in general, and provide the stimulus required to build new research directions toward harnessing metastable phases of promising optoelectronic materials.

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