Title: multiscale modelling of defects in halide perovskites

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Abstract: Perovskites is a class of materials with notable crystal structure of ABX_3, exceptionally wide tunability in chemical compositions and dimensionality in crystal-structures. Due to their exceptional optoelectronic properties, they are widely used for converting and storing (solar) energy, e.g. oxide perovskites as photocatalysts, halide perovskites as absorbers in solar cells, nitride perovskites as mechanical energy harvesters. In these applications, the understanding of optoelectronic properties, chemical stability and their changes upon external stimuli (light excitation, mechanical, thermal and chemical stress) are paramount.

In this talk, I will show how our research group investigate these properties using atomistic multiscale modelling by combing electronic structure calculations with reactive molecular dynamics simulations. Her focus is on halide perovskites and the impact of defects on the efficiency and the stability of perovskite solar cells. We identify harmful defects which lead to either recombination losses and/or chemical degradations and show several strategies to mitigate and passivate these defects. These include engineering the composition of perovskite absorbers, optimizing interfaces with contact materials, and finetuning growth conditions. The atomistic insights provide a basis for further improving the efficiency and stability of perovskite materials and devices. The multiscale computational framework can be enhanced with The emerging data-driven approach and straightforwardly applied to other materials and applications.