**Title of the talk:  Energy Materials: Atomic-scale Insights from *ab initio* modeling**

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**Abstract:** On a global scale, clean energy generation and its efficient use are important aspects to meet rising energy demands with sustainability. However, complex and interdependent structure-property-performance relations strongly limit the directed search and discovery of efficient materials for targeted energy applications. To tackle these challenges, I apply cutting-edge computational simulations that are invaluable to understand and manipulate the functionalities and performances of a wide range of energy materials. In this talk, first I will discuss the details of charge carrier dynamics and structural stability of metal halide perovskites that are leading contenders for next-generation optoelectronic devices. Using non-adiabatic molecular dynamics, I will illustrate the complex influences of dynamic structures on the excited-state carrier dynamics that strongly impact the optoelectronic performances of these materials.[1-4] I will further discuss our work on *in-silico* guided compositional engineering technique that increases the thermodynamic stability and substantially suppresses the anion-migration in halide perovskites.[5] The other part of the talk will briefly focus on the low-dimensional materials that are promising for optical emission and energy-efficient spintronic and nanoelectronic devices.[6,7] I will discuss the potential of small magnetic molecules and layered materials for spin-current generation and transport in nano-device architecture. The impact of dynamic surface on the optical properties of nanocrystals will be another topic of my discussion.[8] In conclusion, I will briefly outline our multidisciplinary future research plans that concentrate on building up reliable computational simulation schemes for fast-tracking systematic designing, optimization, and discovery of materials, highly desirable for various energy technologies.

**References:**

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5. Ferdani *et al. Energy Environ. Sci.* **2019**, 12, 2264-2272
6. Ghosh et al. *Appl. Phys. Lett*. **2015**, 106, 193105
7. Ghosh et al. *Phys. Rev. B*. **2015**, 195136
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Venue: AB2 5B (Offline)

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