Materials Research Seminar

Texas Center for Superconductivity at the University of Houston

Center for Integrated Bio and Nano Systems

Promises and Challenges in Designing Metal-Organic Chalcogenides for Optoelectronic Applications

October 18, 2024

Face-to-face only: 1:30 – 2:30 pm

Location: HSC 102

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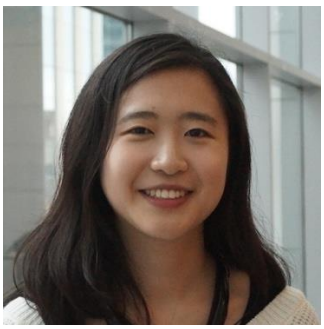
Abstract:



Metal-organic chalcogenides (MOCs) are an emerging class of hybrid materials composed of both organic and inorganic components. The optical processes in the inorganic component of a MOC can be finely tuned by modifying the organic component. A thorough understanding of the optical properties of MOCs is crucial for designing MOCs with desired properties for optoelectronic applications. We explored how the dimensionality, structure, and optical properties of MOCs can be controlled through organic components. The challenges in understanding the structure-property relationship and establishing design principles for these materials will be discussed. A major obstacle lies in the prohibitive computational cost associated with calculating excited state properties. To address this, we developed a cost-effective approach for calculating the absorption spectra of nanomaterials. Our method employs a simplified GW approximation and the Bethe-Salpeter equation, reducing storage requirements to grow quadratically and computational time to grow cubically with system size. It enables the calculation of absorption spectra for nanocrystals and large dye molecules using limited computing resources. Initially applied to finite systems, our method can be extended to periodic systems, offering valuable tools for MOC discovery.

Bio: Dr. Yeongsu Cho received her PhD degree in Chemistry at Columbia University and completed postdoctoral research at MIT. In 2024, she began her independent research group as an assistant professor in the Department of Chemistry at the University of Houston. Her research focuses on the electronic and optical properties of hybrid organic-inorganic materials, development of cost-effective methods for simulating excited state properties of materials, and investigation of electron-phonon coupling effects on these properties.