Moments in Materials Seminar:

Optical properties of the layered perovskites derived from properties of the bulk perovskites

Speaker: Yeongsu Cho, Columbia University
When: Friday, May 15th, 2020, 4:00 pm
Where: Register for link: https://columbiauniversity.zoom.us/meeting/register/tJIldeurrT8jE9b6L2i4oU4yoP_5A669tX-J

Lead-halide perovskite is one of the promising candidates for solar cell absorbers, owing to the high extinction coefficient, and the band gap of the visible range, showing a high power conversion efficiency reported above 25%. A major weakness of lead-halide perovskite is that they are intrinsically unstable to moisture, air, and light, which prevents it from being commercialized. One of the solutions is to replace the cation to a bulky organic molecule to form a layered structure of hybrid organic-inorganic halide perovskites (HOIP) that are stable under working conditions. To maximize the performance of the layered HOIP, a comprehensive understanding of the optoelectronic properties of perovskites is required. However, a fully ab-initio calculation of layered HOIPs is computationally prohibitive due to a large number of atoms in a unit cell. I will talk about a semi-classical method that allows investigating the properties of layered HOIPs using the properties of bulk HOIPs, capturing essential physics with an affordable computational cost. The tight-binding approximation is employed to calculate the electronic properties, parametrized by first-principles calculations. Electrostatic screening is classically treated to correctly describe the effect of the heterogeneous dielectric environment of layered HOIPs. Our method calculates the optical spectra of layered HOIPs that are in good agreement with those from the reported experiments and shows a transition of the electronic and optical properties from quasi-two-dimensional to three-dimensional behavior.