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Defect and dynamic properties of perovskite halides from first principles

Dr. Maria Chan

Center for Nanoscale Materials,
Argonne National Lab, Illinois, U.S.A.

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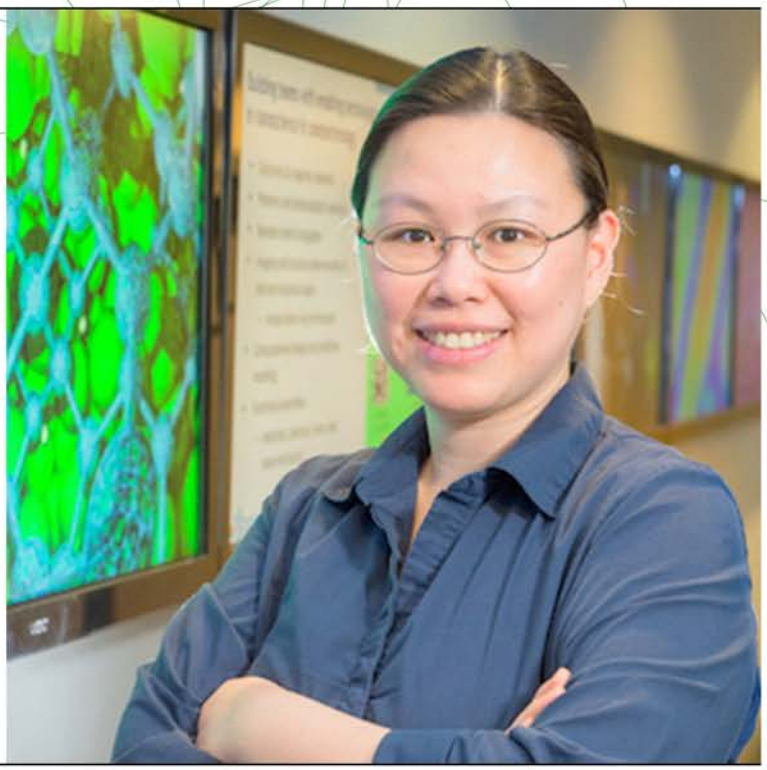

Hybrid organic-inorganic perovskite halides have been intensely investigated due to their exemplary properties for diverse optoelectronic applications including photovoltaics. An understanding of the design of hybrid perovskites can benefit significantly from density functional theory (DFT) and machine learning approaches. In this talk, we will discuss (1) electronic properties of methlyammonium lead halide (MA-Pb-halide) perovskites having different cation and halide compositions with various defects and impurities, obtained using first principles DFT calculations and machine learning; (2) dynamics of lattice thermal equilibration, especially between the organic and inorganic sublattices, from ab initio molecular dynamics simulations.

We will also discuss the availability of computational resources and staff scientist expertise at Nanoscale Science Research Centers funded by the United States Department of Energy.

Participants are required to register in advance for this meeting here:

https://us02web.zoom.us/meeting/register/tZAsc-mrpzgoE9dSiS1q8yOe0CqBYone9Bwi

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