Optoelectronic Properties of Halide Perovskites at Finite Temperature

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Halide perovskites (HaPs) are promising materials for applications in energy and optoelectronic devices owing to their fascinating microscopic properties. Of particular scientific interest is the coupling of electronic to lattice-dynamical properties of HaPs that occurs at finite temperature, because the vibrational properties of the compounds exhibit multiple fascinating effects, such as anharmonicity, dynamic disorder and localization. These challenge our basic understandings of charge-carrier and optical characteristics of these compounds. In this talk, I will present our recent theoretical findings obtained from molecular dynamics simulations based on density functional theory, in order to discuss intriguing confluences of unusual vibrational and optoelectronic effects. It will be shown that the rather special vibrational characteristics of HaPs might not just be a mere coincidence, but play active roles in establishing their favorable properties.