Effect of anharmonicity on optoelectronic properties of semiconductors

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In our work, we are particularly interested in scenarios where atoms in semiconductors show strong structural dynamical effects such as anharmonic vibrations. These effects trigger many puzzling questions in regard to updated structure-property relations and improved theoretical understandings of these solids. They also motivate a number of exciting theoretical developments needed for predicting materials properties in the presence of disorder.

In my talk, I will present our recent findings regarding theoretical treatments of structural dynamics in semiconductors and how we may use them to improve our understanding of their finite-temperature properties. The results will focus on halide perovskite and nitride semiconductors,[1-4] demonstrating the impact of anharmonic vibrations on optoelectronic properties such as band gaps and carrier mobilities.

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