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Effect of Lattice Screening on Excitonic and Optical Properties in $CH_3NH_3PbI_3$ Solar Cell Materials[1] JOSHUA LEVEILLEE, ANDRE SCHLEIFE, Univ of Illinois - Urbana, ANDRE SCHLEIFE RESEARCH GROUP TEAM — Hybrid Organo-Metallic Perovskites have made great strides towards becoming a next generation solar cell material. Though high performing experimental devices have been constructed from these perovskites, the fundamental optical and electronic physics of these systems remains an active area of research. A large lattice dielectric constant in the Methylammonium(CH_3NH_3)-Lead(Pb)-Iodide(I_3) system potentially contributes to the screening of the electron-hole interaction. The strongly increased dielectric screening due to lattice contributions has been suggested to reduce the exciton binding energy and strongly effects the optical band gap. In this study, we seek to understand, from first principles, the interplay between lattice screening and exciton binding energy. We use density functional theory for ground state calculations and the Bethe-Salpeter equation for the optical polarization function, from which we calculate optical spectra and excitonic properties. We will discuss differences between lattice and electronic screening and the effect on the optical properties of multiple $CH_3NH_3PbI_3$ phases.

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