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Exploring various sources of electron-hole screening in $CH_3NH_3PbI_3$ solar cell materials using the Bethe-Salpeter equation[1] JOSHUA LEVEILLEE, ANDRE SCHLEIFE, University of Illinois, Urbana-Champaign — Hybrid organic-inorganic perovskite materials have emerged as promising next generation thin-film solar cells. While many working devices have been developed, the weak electron-hole interaction and low exciton binding energy have not been fully explained. Methods beyond ground-state calculations are required to fully understand the excited state properties of these materials. In this work, the excitonic spectrum of $CH_3NH_3PbI_3$ is simulated using the Bethe-Salpeter Equation. We describe contributions to dielectric screening, such as electronic, free-carrier, lattice, and polaron, through the use of model dielectric functions for the electron-hole Coulomb interaction. The calculated optical properties are directly compared, qualitatively and quantitatively, to experimental results. We find that the contributions of lattice and free carrier screening are highly influential on the optical spectrum.

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