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Design of photo-absorption properties of hybrid organic-inorganic halide perovskite photovoltaic devices by cation manipulation[1] OSCAR GRANAS, SEAS, Harvard University and Dept. of Physics and Astronomy, Uppsala University, DMITRY VINICHENKO, Dept. of Chemistry and Chemical Biology, Harvard University, EFTHIMIOS KAXIRAS, Dept. of Physics, Harvard University — Photovoltaic devices based on hybrid organic-inorganic halide perovskite materials have lately sailed up as one of the most promising technologies for cost effective harvest of solar energy. In just a few years the efficiency has surpassed that of both conventional dye-sensitized- and organic solar cells. In this study we investigate the influence of the size of the cationic π-system on the electronic and structural properties of the perovskite photo-absorbing material. Using theoretical simulations we investigate key quantities for photovoltaic efficiency, such as band-gap, electron- and hole mass. We show that by changing the cation the band-gap and effective masses can be controlled. Structural changes are addressed, where we can see an enhanced influence of dispersion interaction as the cation polarizability increases. The effects of spin-orbit coupling is considered for both structural and electronic properties.

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