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**Electronic properties of perovskite absorbers for solar cell applications**[1] MARINA FILIP, FELICIANO GIUSTINO, University of Oxford, Department of Materials — Metal halide perovskite absorbers have captured the attention of the photovoltaics research community in the past 3 years, reaching efficiencies over 19%. Despite this unprecedented progress, the remarkable physical properties of these materials are not yet fully understood. In this work we show an exhaustive computational study of $CH_3NH_3PbI_3$ within density functional theory and the GW approximation. We show the effect of semicore states and spin-orbit coupling on the quasiparticle band gap of $CH_3NH_3PbI_3$ and describe a straightforward "self-consistent scissor" method to correct the underestimated dielectric screening in the G0W0 approach [1]. Finally, we model the interplay between the structural and electronic properties of lead-iodide perovskites and propose novel lead-iodide peroskite absorbers with different cations at the center of the cuboctahedral cavity facilitating the tunning of the fundamental band gap [2].

[1] Filip, M. R. & Giustino, F., http://arxiv.org/abs/1410.2029 (2014)
[2] Filip, M. R., Eperon, G., Snaith, H. J. & Giustino, F., http://arxiv.org/abs/1409.6478 (2014)

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