Electronic properties of perovskite absorbers for solar cell applications\textsuperscript{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\textsubscript{3}NH\textsubscript{3}PbI\textsubscript{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\textsubscript{3}NH\textsubscript{3}PbI\textsubscript{3} and describe a straightforward “self-consistent scissor” method to correct the underestimated dielectric screening in the G0W0 approach \cite{Filip2014}. Finally, we model the interplay between the structural and electronic properties of lead-iodide perovskites and propose novel lead-iodide perovskite absorbers with different cations at the center of the cuboctahedral cavity facilitating the tuning of the fundamental band gap \cite{Filip2014b}.

\textsuperscript{1}This work was supported by the ERC (EU FP7 / ERC 239578), UK EPSRC (EP/J009857/1) and the Leverhulme Trust (RL-2012-001).

\begin{thebibliography}{9}
\end{thebibliography}