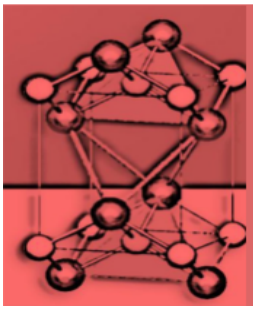

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# Simulation of Hybrid Metal Halide Perovskites

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Hybrid metal halide perovskites with organic A-site cations have made a great impact in solar cell research, as well as other areas. Here, I present some fundamental aspects of the simulation of these materials using density functional theory, together with our research. These studies include several aspects of single phase $MAPbI_3$ ($MA{=}CH_3NH_3$), ferroelectric-like grain boundaries, and interfaces with a hole transport material. Also, I present a model of a solid solution of $FAPbI_3$ with $MAPbBr_3$, where $FA{=}HC(NH_2)_2$.