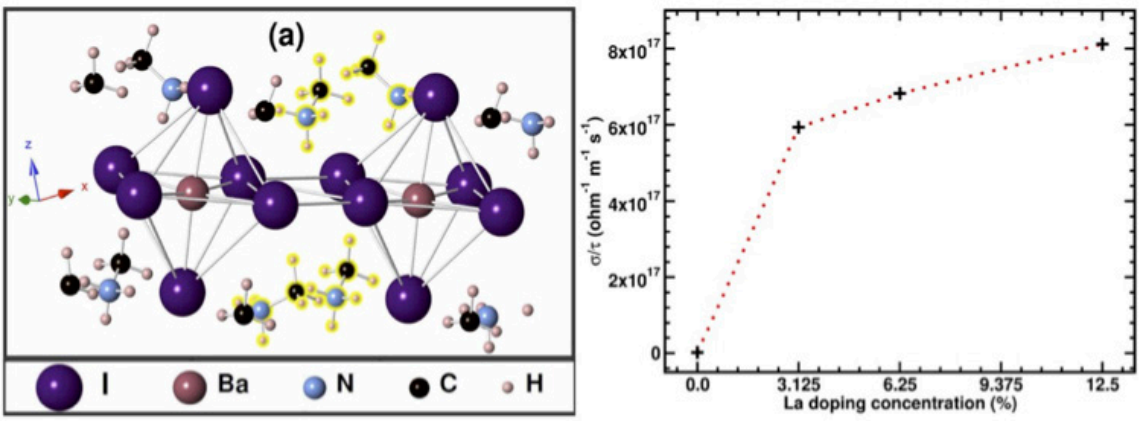
Discovering new transparent conducting material

Hybrid perovskites, $CH_3NH_3PbI_3$ (crystal structure shown on the left figure), is one of the most promising novel materials for solar harvesting. Toxicity of lead (Pb), however, has always remained a concern. In this project, we investigated the electronic structure of complete replacement of Pb by alkaline earth elements (Ca, Sr, Ba) and found them to be wide band gap (E_g) semiconductors (band gap ~ 3.7-4 eV), and hence not suitable as absorber material. This opens up a new avenue to explore these materials as transparent conductor (TC). We doped $CH_3NH_3PbI_3$ (largest E_g) with La, which shifts its Fermi level (EF) at conduction band bottom and induces states at EF for conduction. This is precisely what is required for transparent conductors. Optical and transport properties simulated from linear response [within Density Functional Theory (DFT)] calculations suggested it to be a very good TC material with a high figure of merit (sigma/a) (shown in right panel of the above figure), where 'sigma' is the electrical conductivity and 'a' is the optical absorption coefficient. This claim is also supported by our calculated results on density of states at EF, effective mass, carrier concentration etc. at various La-doping. We propose $CH_3NH_3(Ba1\text{-}xLax)I_3$ (x<12.5%) to be a good TC material to be used in an all perovskite solar



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