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# The Effect of the Surface Composition on Electronic Properties of Methylammonium Lead Iodide Perovskite

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**Abstract**: Methylammonium lead iodide perovskite, $CH_3NH_3PbI_3$, is one of the most promising photovoltaic materials for low-cost and clean source of energy. In this work, the first-principles calculations were carried out to investigate the different composition of $CH_3NH_3PbI_3$ (001), including both methylammonium iodide terminated (MAI-T) and $PbI_2$ terminated ($PBI_2$-T) surfaces. The calculated surface energies show that the MAI-T is thermodynamical more stable than the $PBI_2$-T one under the equilibrium growth condition. The electronic properties of the two types of surfaces are also different. The band gap of $PBI_2$-T is obviously smaller than that of MAI-T due to the surface Pb states. Band gaps of MAI-T decrease with increasing thickness, while band gaps of $PBI_2$-T are insensitive to the slab thickness. The calculated optical absorption coefficients suggest that both terminations are effective solar energy absorbers in the visible light spectrum.