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Structural Stabilities and Electronic Properties of High-Angle Grain Boundaries in Perovskite Cesium Lead Halides. YAGUANG GUO, Peking University — Organometal trihalide perovskites are emerging as very promising photovoltaic materials, which is rivaling that of single crystal silicon solar cells despite their polycrystalline nature with relatively high density of grain boundaries (GBs). There is a lack of understanding of the effects of GBs on halide perovskites as their presence in silicon and other photovoltaic materials is generally determinated to their photovoltaic properties. Using first-principles calculations, we systematically investigate the geometric structures of high-angle tilt GBs in halide perovskites CsPbX3 (X = Cl, Br, and I) by the coincidence site lattice (CSL) model and mapping their γ surfaces. We show that, after crystal shift, $\Sigma5(210)(0.4,0)$ is proved to be most stable among all the GB models. Electronic properties calculations further reveal that, different from the class GB model, GBs in halides perovskites have no harmful effects on optoelectronic properties of the bulk phase because of the large distance between the unsaturated atoms and the atomic reconstruction in the GB region. We also extend the results to MAPbI3 GBs and also show their benign effect on optoelectronic properties.

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