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Thermal stability of organic-inorganic hybrid perovskite structures from first principles AMIR FARAJIAN, Department of Mechanical and Materials Engineering, Wright State University — Organic-inorganic hybrid perovskites are currently the focus of intense research owing to their impressive efficiency as photovoltaic devices. Specifically, methylammonium lead tri-halides are of interest in this regard, however, some of their basic properties are not completely known yet. We investigate structural stability of organic-inorganic hybrid perovskites of methylammonium lead tri-halide type ($MAPbI_{3-n}Cl_n$: n = 0-3) at different temperatures, using ab initio structure optimization, energy calculations, and molecular dynamics. Different crystal structures and free energies are compared, and effects of temperature change are discussed. The results provide insight toward understanding stable methylammonium lead tri-halides for photovoltaic applications.

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