Towards a pressure-temperature phase diagram of organo-halide hybrid perovskite from *ab initio* molecular dynamics

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Abstract:

Recently, there has been a growing interest in a new class of solar cells based on organo-halide lead perovskite due to their superior photovoltaic performances [1,2]. Methyl amine lead bromide perovskite ($MAPbBr_3$) is one of them, having different stable phases (*Pm$\bar{3}$m, Im$\bar{3}$, Pnma* etc.) at different temperature and pressure conditions [3,4]. In this work we employ *ab initio* molecular dynamics to obtain equilibrium structural properties of different phases and describe the reasons of stability of those phases at different temperature and pressure conditions. We also explore the correlations between the ordering of methylamine dipoles in different phases and the distortion of Pb-Br lattice by defining suitable order parameters.

Figure:

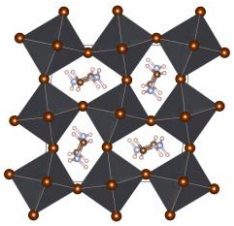

Fig: Structure of Pnma phase of $MAPbBr_3$

References and Notes:

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2. Kojima, Akihiro, et al. "Organometal halide perovskites as visible-light sensitizers for photovoltaic cells." *Journal of the American Chemical Society* 131.17 (2009): 6050-6051.
3. Swainson, I. P., et al. "Pressure response of an organic− inorganic perovskite: methylammonium lead bromide." *Chemistry of materials* 19.10 (2007): 2401-2405.
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Bio-Sketch of Speaker

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