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Elucidating the degradation of methylammonium lead iodide perovskite ($CH_3NH_3PbI_3$) at high temperatures and humid conditions via molecular dynamics simulations with ab initio force fields OMOLOLU AKIN-OJO, Theoretical Physics Department, African University of Science and Technology — In recent times, the efficiencies of lead halide perovskite solar cells have soared to more than 15% and there is a potential for further increase. However, these solar cells degrade quickly when exposed to heat and moisture. This degradation limits the large scale production of the device. In this work we use molecular dynamics simulations to study $CH_3NH_3PbI_3$ when exposed to high temperatures ($30 - 80°C$) and water. The force fields used in the simulations were determined from ab initio calculations on the system. The structural changes that occur in methylammonium lead halide perovskite under conditions of high temperature and humidity will be inferred from the simulations.

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