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Dynamics of CH3NH3PbI3 from first principles simulations[1] ALI KACHMAR, MARCELO CARIGNANO, Qatar Environment and Energy Research Institute, Qatar Foundation, PO Box 5825, Doha, Qatar — We address the dynamical and optical properties of CH3NH3PbI3 using molecular dynamics simulations based on forces calculated with density functional theory. We have studied the three stable phases of CH3NH3PbI3 but most of the effort was dedicated to the intermediate tetragonal phase, which is stable at standard ambient conditions. In this case, two different system sizes have been considered, one with 8 unit cells (384 atoms) and a larger one with 27 unit cells (1296 atoms). The total simulated time reached 40 ps. Our findings reveal the interplay between the thermal energy of the system and the electronic degrees of freedom. For example, the organic molecule undergoes relatively fast rotations and the energy band gap, approximated by the LUMO-HOMO energy difference, fluctuates around the equilibrium value of $\sim$1.5 eV with a width of 0.2 eV. The rotation of the CH3NH3 molecule is not isotropic, and more importantly, it is quite sensitive to the size of the simulation box. Our study also provides a quantitative measure for the finite size effects affecting the calculated properties and provides a contextual scenario on which to analyze the more typical density functional theory studies based on static calculations on optimal structures.

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