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Rotational Dynamics of Organic Cations in $CH_3NH_3PbI_3$ Perovskite TIANRAN CHEN, BENJAMIN FOLEY, Univ of Virginia, BAHAR IPEK, Univ of Delaware, MADHUSUDAN TYAGI, JOHN COPLEY, CRAIG BROWN, NCNR, JOSHUA CHOI, SEUNG-HUN LEE, Univ of Virginia — Methylammonium lead iodide ($CH_3NH_3PbI_3$) based solar cells have shown impressive power conversion efficiencies of above 20%. However, the microscopic mechanism of the high photovoltaic performance is yet to be fully understood. Particularly, the dynamics of $CH_3NH_3^+$ cations and their impact on relevant processes are still poorly understood. Using elastic and quasi-elastic neutron scattering techniques and group theoretical analysis, we studied rotational modes of the $CH_3NH_3^+$ cation in $CH_3NH_3PbI_3$.[1] Our results show that, in the cubic and tetragonal phases, the $CH_3NH_3^+$ ions exhibit four-fold rotational symmetry of the C-N axis (C_4) along with three-fold rotation around the C-N axis (C_3), while in orthorhombic phase only C_3 rotation is present. Around room temperature, the characteristic relaxation time for the C_4 rotation is found to be 5ps while for the C_3 rotation is 1ps. The T-dependent rotational relaxation times were fitted with Arrhenius equations to obtain activation energies. Our data show a close correlation between the C_4 rotational mode and the temperature dependent dielectric permittivity. Our findings on the rotational dynamics of $CH_3NH_3^+$ and the associated dipole have important implications on understanding the low exciton binding energy and slow charge recombination rate in $CH_3NH_3PbI_3$ which are directly relevant for the high solar cell performance. [1] T. Chen et al., Phys. Chem. Chem. Phys., 2015, DOI: 10.1039/C5CP05348J.

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