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Origin of low thermal conductivity in organic-inorganic thermoelectric materials TOMOYUKI HATA, Department of Chemical System Engineering, School of Engineering, The University of Tokyo, GIACOMO GIORGI, Dipartimento di Ingegneria Civile e Ambientale, Universit degli Studi di Perugia, KOICHI YAMASHITA, Department of Chemical System Engineering, School of Engineering, The University of Tokyo — Hybrid organic-inorganic halides have recently attracted attention as thermoelectric materials due to their low thermal conductivity, which still remains unexplained. There are many possible factors at the origin of phonon scattering, and the attribution of the low thermal properties to such factors is an inevitable issue to control and design the hybrid thermoelectric materials. In this study, we adopt $CH_3NH_3PbI_3$ (hereafter MAPI) as organic-inorganic halide species and perform the mentioned attribution by combining classical and *ab-initio* calculations. At first, we have developed an empirical potential for MAPI. Bond, angle, and dihedral potential functions are expanded to higher-order to include anharmonicity and fitted to the force trajectories of the *ab-initio* molecular dynamics calculations. By using our force fields, we calculate the thermal conductivity of MAPI by means of the reverse non-equilibrium molecular dynamics method. The results are in very good agreement with the experimental thermal conductivity. We investigate the origin of such transport properties by changing the degrees of freedom of the embedded MA molecular cations and by evaluating the relaxation paths based on the velocity autocorrelation functions.

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