Low energy phonon spectroscopy and translation-rotation coupling in hybrid perovskites crystals

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Despite the wealth of research conducted the last three years on hybrid organic perovskites (HOP), several questions remain open including: to what extend the organic moiety changes the properties of the material as compared to all-inorganic (AIP) related perovskite structures. To ultimately reach an answer to this question, we have recently introduced two approaches[1,2] that were designed to take the stochastic molecular degrees of freedom into account, and suggested that the high temperature cubic phase of HOP and AIP is an appropriate reference phase to rationalize HOP's properties. In this paper, we recall the main concepts and show recent molecular dynamic results (figure 1) to discuss more specifically the various possible couplings between charge carriers and low energy excitations such as acoustic and optical phonons. As available experimental or simulated data on low energy excitations are limited, we also present preliminary neutron and Brillouin scattering, as well as ultrasonic measurements obtained on freshly prepared single crystals of $CH_3NH_3PbBr_3$.

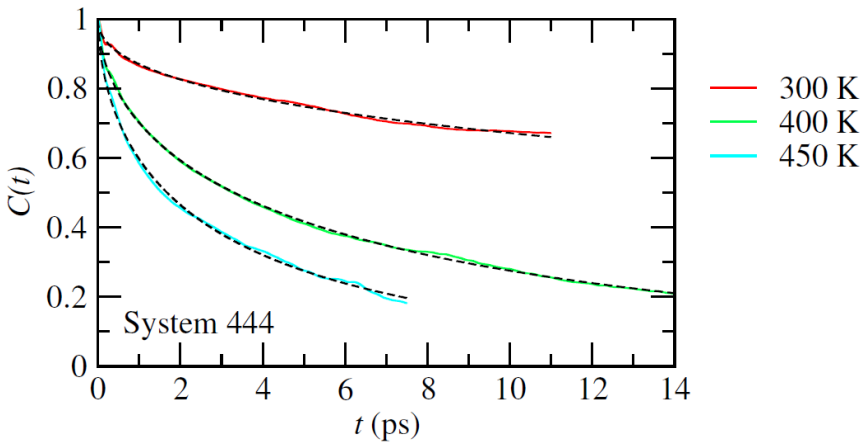

Figure 1. Temperature dependence of the average autocorrelation function of the CN axis orientation in MAPbI3 extracted from first principles MD simulations for a 444 cubic supercell (solid lines): (top) 300K, (middle) 400K and (bottom) 450K. Dashed lines are fits using stretched exponential functions.

[1] Even, J. J. Phys. Chem. Lett. 6, 2238–2242 (2015).
[2] Even, J., Carignano, M. and Katan, C., Nanoscale (2016), doi: 10.1039/C5NR06386H.

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