

Supporting information to

Tuning the thermal conductivity of methylammonium lead halide by the molecular substructure

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Table T1: Lattice thermal diffusivity $\bar{\kappa}$ and conductivity κ for $L_z=25$ nm

calculation	$\bar{\kappa}(T=300\text{ K})$ ($10^{-7}\text{ m}^2/\text{s}$)	$\kappa(T=300\text{ K})$ (W/mK)
standard AEMD	0.98 ± 0.20	0.20 ± 0.04
torque = 0	0.89 ± 0.18	0.17 ± 0.03
rigid NH ₃	0.70 ± 0.13	0.12 ± 0.02
rigid CH ₃	1.05 ± 0.21	0.18 ± 0.04
rigid CH ₃ and NH ₃	1.34 ± 0.23	0.16 ± 0.03
rigid MA	3.20 ± 0.61	0.31 ± 0.06
rigid MA, torque = 0	3.86 ± 0.73	0.35 ± 0.07

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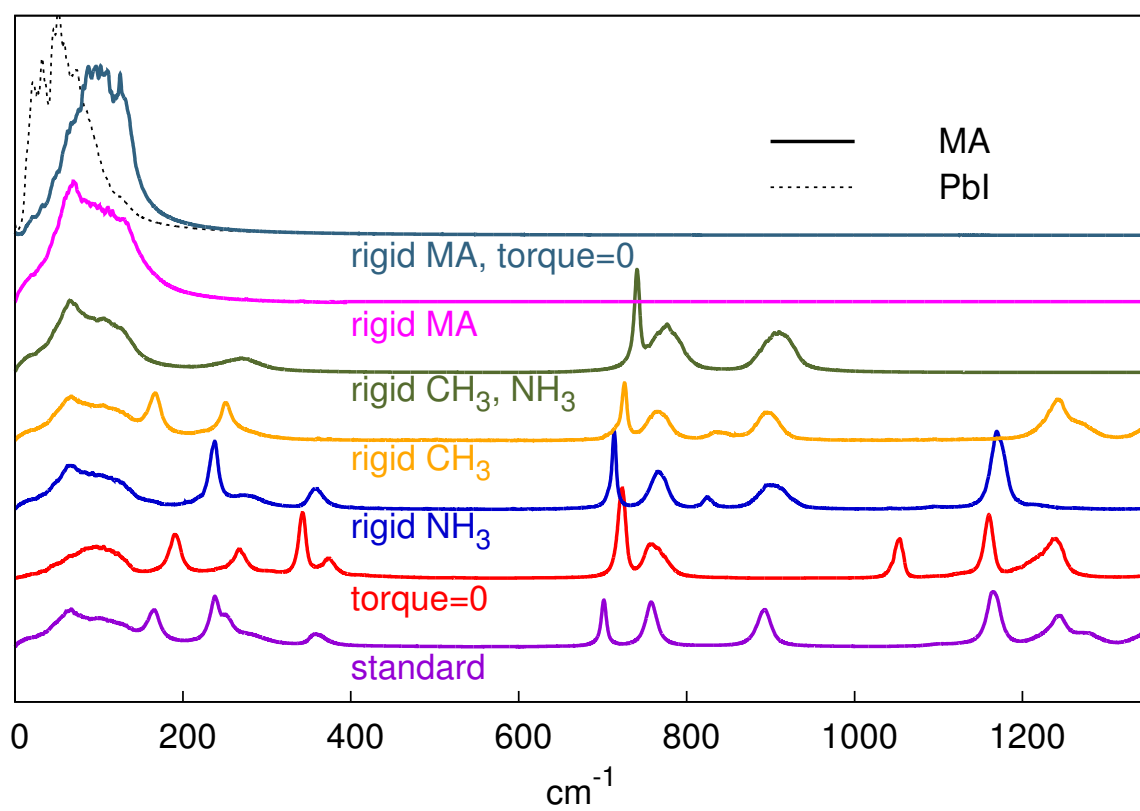


Figure S1: VDOS of MAPI up to $\sim 1300 \text{ cm}^{-1}$