Computational Design of Hybrid Perovskites for Highly Stable and Flexible Energy-Related Devices

- **Hybrid** perovskite $CH_3NH_3PbI_3$ ($MAPbI_3$) merges as promising energy-related (i.e., photovoltaic, LED, and thermoelectric) materials.
- **Orthorhombic** and tetragonal $MAPbI_3$ show strong elastic anisotropy, while cubic $MAPbI_3$ shows weaker elastic anisotropy due to its higher structural symmetry (**Figure 1**).[a]
- **$MAPbI_3$** possesses significant plastic deformation (glassy) region after the initial elastic deformation, originated from its soft and nano-ductile nature (**Figure 2**).[a] Coulombic attractions dominate the total ionic interactions.

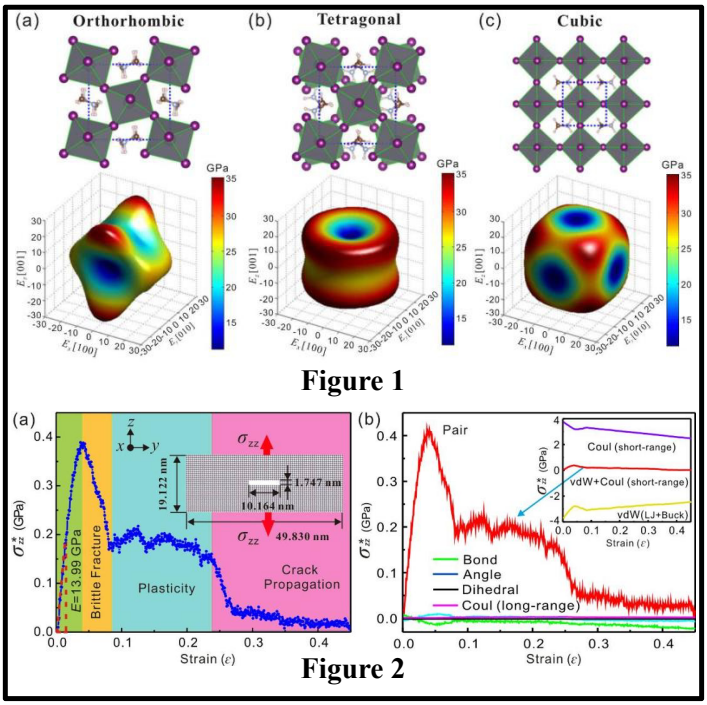

Figure 1

Figure 2

- **$MAPbI_3$** has ultralow thermal conductivity (< 1 $Wm^{-1}K^{-1}$), and as low as 0.31 $Wm^{-1}K^{-1}$ at room temperature. Electrostatic interactions dominate total thermal transport in $MAPbI_3$ (**Figure 3**).[b]
- **The** anisotropy in thermal conductivity at lower temperatures associates with preferential orientation of organic MA+ cations (**Figure 3**).[b]
- **Ultralow** thermal conductivity results from the small phonon group velocities due to low elastic stiffness, short phonon lifetime and mean free path due to the phonon-phonon scattering (**Figure 4**).[b]
- **Thermal** conductivities of hybrid perovskites $MABX_3$ (B = Pb, Sn; X = I, Br) can be qualitatively predicted by the simple relation (**Figure 5**):[b]

$$\kappa \sim v_{avg}^2 \sim (v_L^2 + v_T^2)/2 \sim M/\rho \quad (M = (E + G)/2)$$

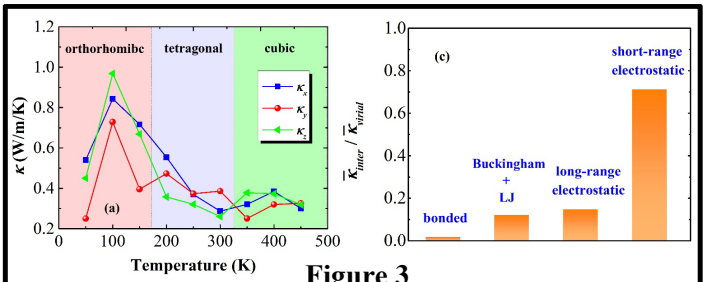

Figure 3

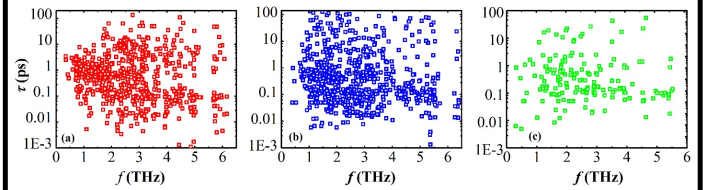

Figure 4

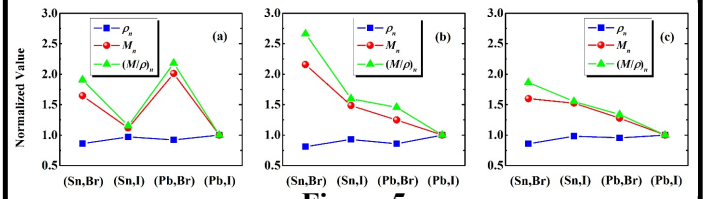

Figure 5

Future Directions:

- **Predict** the surface stability and lifetime of hybrid perovskites against high temperature, moisture, and direct water contact.
- **Understand** the solution-phase crystallization process of hybrid perovskites in various solvents, physical vapor deposition on substrates, and ion/defect migration under biased electric potentials.
- **Computational** high-throughput screening of emerging hybrid perovskites for next generation thermo-opto-electronics.

[a] M. Wang, S. Lin, "Anisotropic and Ultralow Phonon Thermal Transport in Organic-Inorganic Hybrid Perovskites: Atomistic Insights into Solar Cell Thermal Management and Thermoelectric Energy Conversion Efficiency", ***Advanced Functional Materials***, 2016, in press.

[b] J. Yu, M. Wang, S. Lin, "Probing the Soft and Nano-Ductile Nature of Hybrid Perovskites from Microstructural Evolution and Atomic Stress Decomposition", ***ACS Nano***, 2016, under review.

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