Supporting Information

Unveiling the Strain-Sensitive Thermal Transport Properties of Chlorinated Diamane

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S1. The localized phonon density of states.



Figure S1. The local density of states for A- and B-type carbon atoms and functional groups projected along the in-plane and out-of-plane directions in HD (left), FD (middle), and ClD (right), both with solid lines representing 5%-strained configurations and dashed lines representing unstrained configurations. Moving from top to bottom, the panels depict the in-plane and out-of-plane A-type carbon atom, followed by the in-plane and out-of-plane B-type carbon atom, and finally the in-plane and out-of-plane H/F/Cl atom.