Supplementary information:

Insights into the thermal conductivity of MOF-5 from first principles

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The phonon lifetime τ_λ is calculated based on a perturbation to the non-interacting harmonic modes $\lambda = (q,s)$. We focus our attention on the three-phonon processes whose scattering rate $1/\tau_\lambda$ in the single-mode relaxation time approximation can be computed via

$$\frac{1}{\tau_\lambda} = \pi \sum_{q',s',s''} \left|V_3(s,-q;s',q';s'',q'')\right|^2$$
$$\times \left[\left(1+n_{s'q'}+n_{s''q''}\right)\delta\left(\omega_{s'q'}+\omega_{s''q''}-\omega_{s,-q}\right)+2\left(n_{s''q''}-n_{s'q'}\right)\delta\left(\omega_{s'q'}-\omega_{s''q''}-\omega_{s,-q}\right)\right]$$

where $V_3(s,-q;s',q';s'',q'')$ are the three-phonon coupling matrix elements.

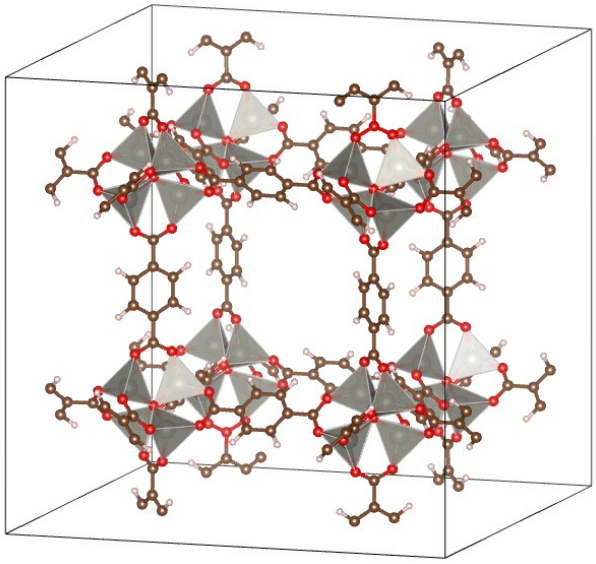

Fig. S1 The optimized crystal structure of MOF-5 in consist of organic linkers and ZnO_4 metal clusters.

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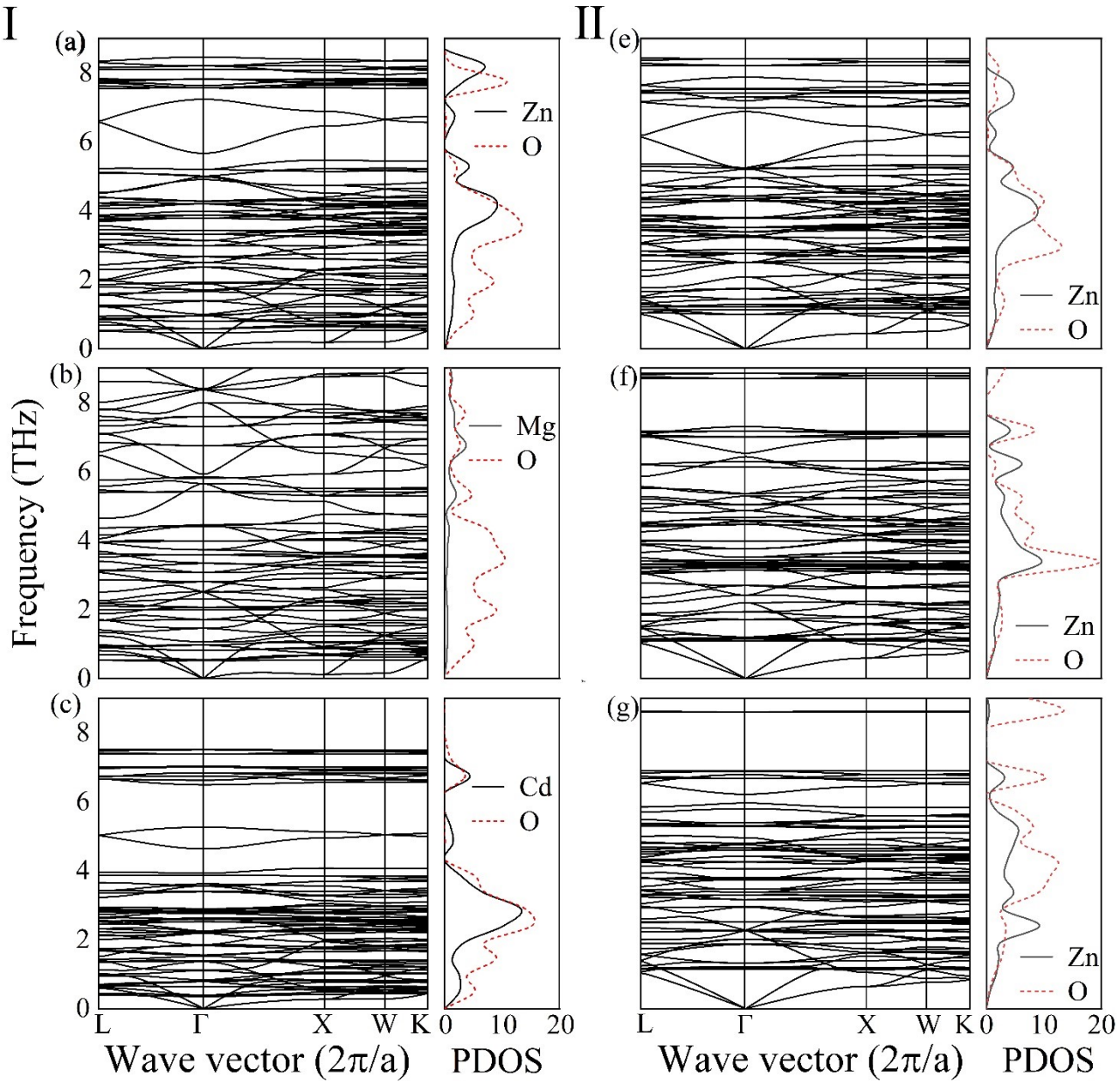

Fig. S2. (I). The phonon dispersion curves and phonon PDOS of MOF-5 with different metals (a) Zn, (b) Mg, and (c) Cd. (II). The phonon dispersion curves and phonon PDOS of MOF-5 under ε of (e) 2%, (f) 4%, and (g) 6%. For clarity, only the low-frequency phonon bands are shown, since phonon dispersion curves above 8 THz are rather flat.