Supporting Information: Coherent phonon transport in 2D layered Cu_3BHT metal organic frameworks

Riccardo Dettori[1,*], David Beljonne[2], Luciano Colombo[1], and Claudio Melis[1]

[1]Department of Physics, University of Cagliari, Monserrato, CA, 09042, Italy
[2]Laboratory for Chemistry of Novel Materials, University of Mons, Mons, Belgium
[*]corresponding: riccardo.dettori@dsf.unica.it

ABSTRACT

Table 1. Interatomic distancies for the three stacking configurations.

	d_{C-C} (Å)	d_{C-S} (Å)	d_{Cu-S} (Å)
AA	1.411	1.715	2.264
AB	1.410	1.721	2.255
C	1.407	1.724	2.264

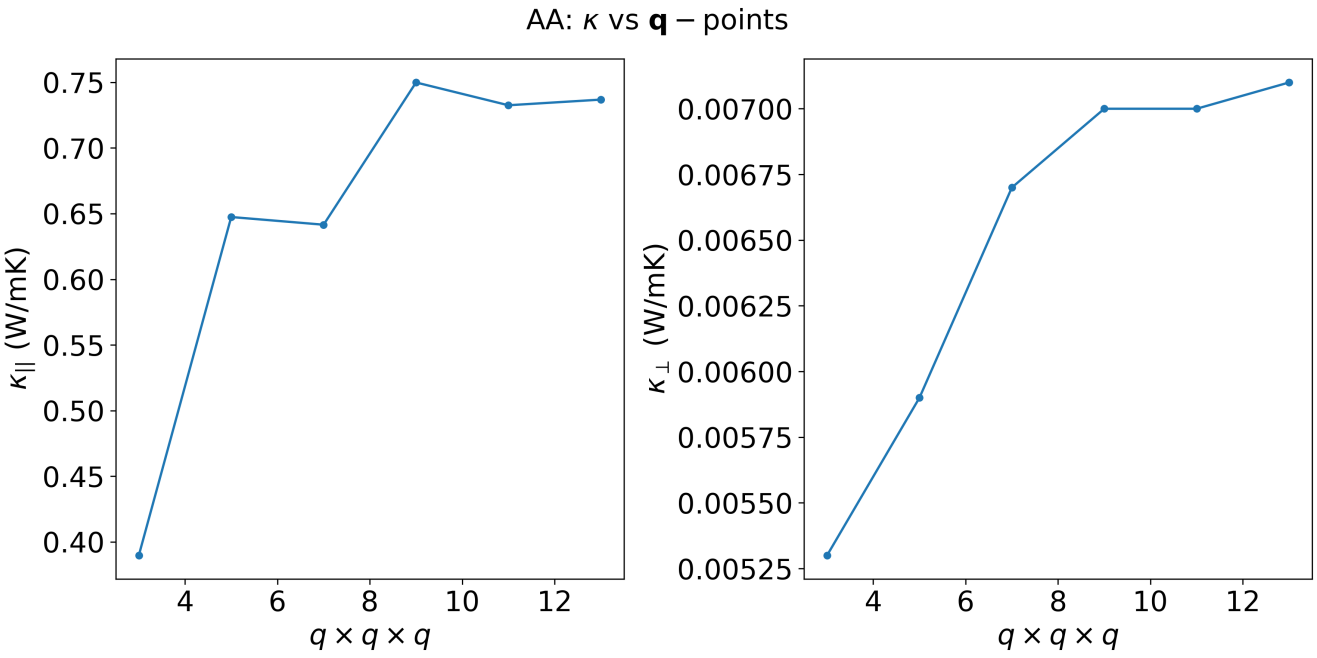

Figure 1. In-plane ad out-of-plane thermal conductivity for the AA stacking as a function of the adopted $\mathbf{q}-$points mesh.

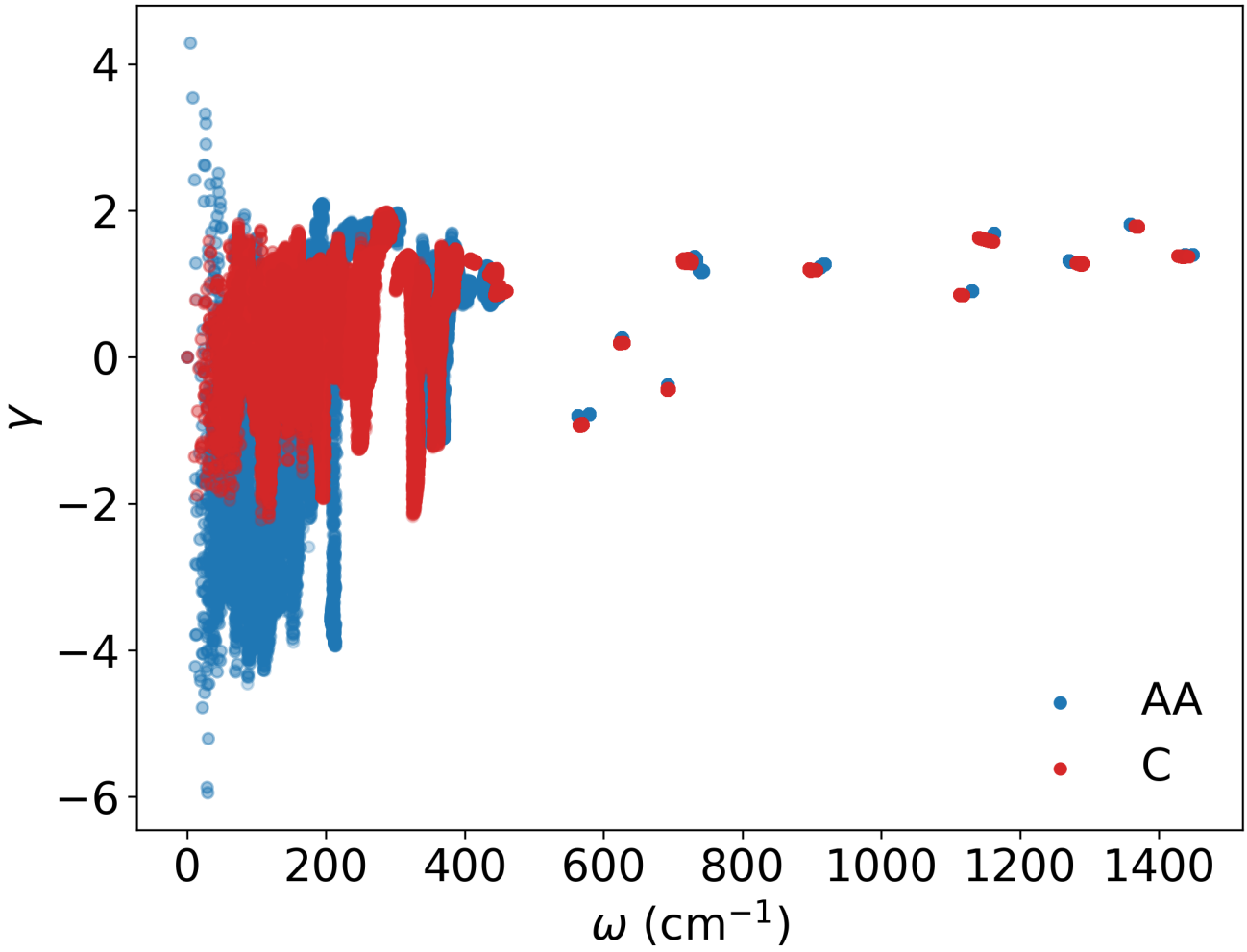

Figure 2. Grüneisen computed for AA and C stacking.

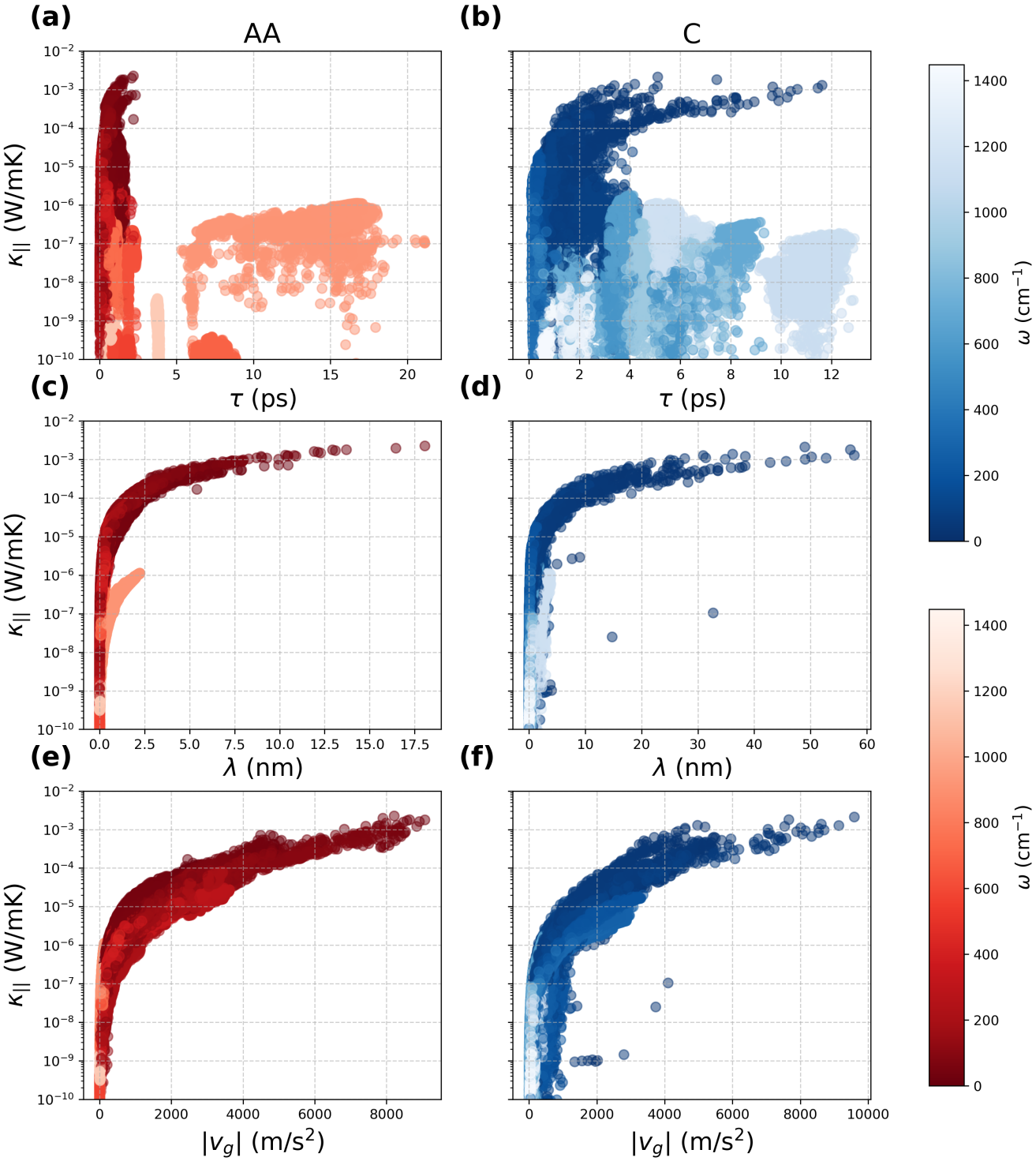

Figure 3. Correlation plots for in-plane thermal conductivity with (a,b) phonon lifetimes, (c,d) phonon mean free paths, and (e,f) group velocity magnitude for AA- and C-Cu_3BHT.

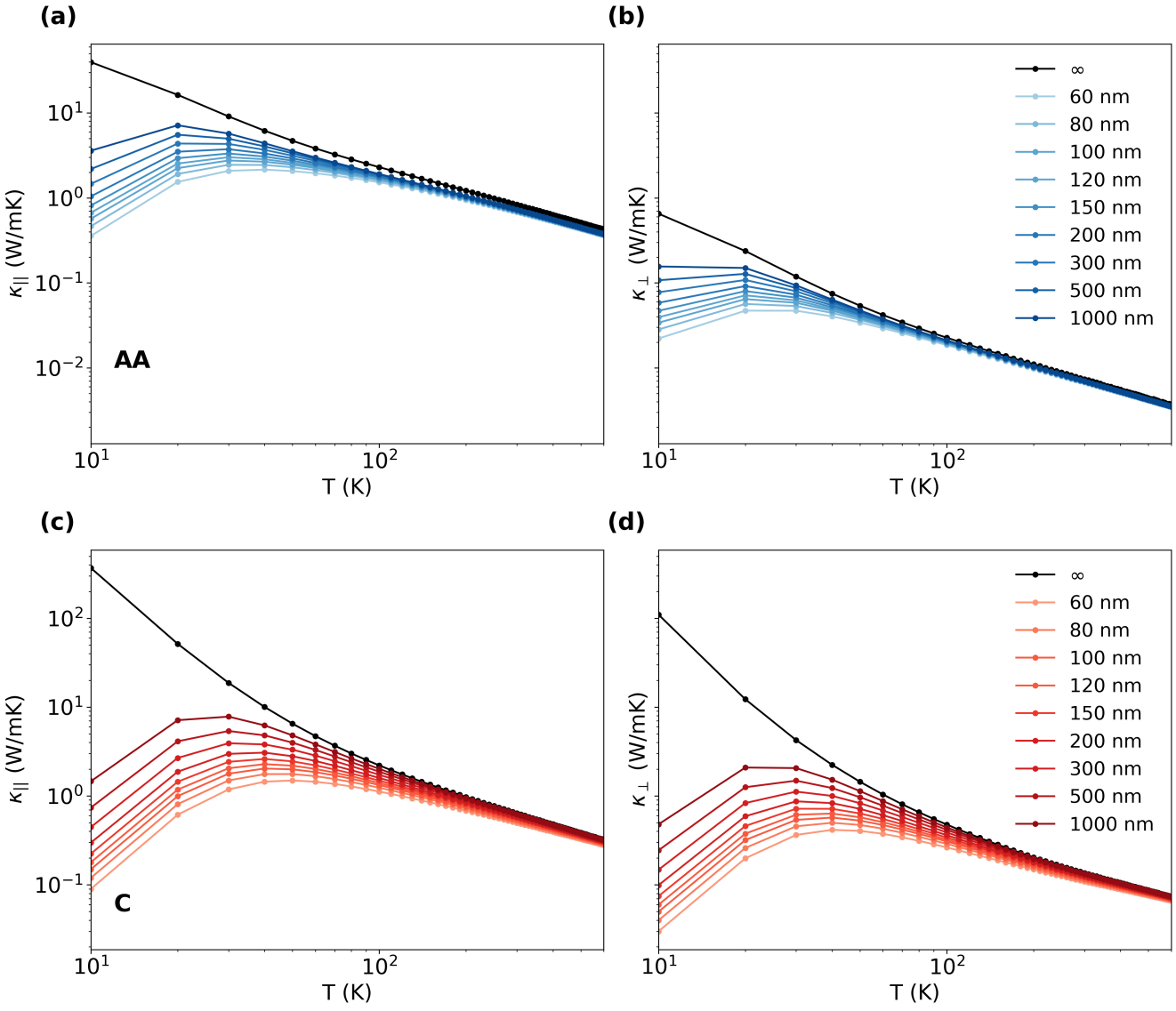

Figure 4. Phonon-boundary scattering-corrected thermal conductivity in both the (a,c) in-plane and (b,d) out-of-plane direction.