Supporting Information

Correlated Missing Linker Defects Increase Thermal Conductivity in Metal-Organic Framework UiO-66

Meiirbek Islamov[1], Paul Boone[1], Hasan Babaei[2], Alan J. H. McGaughey[3], Christopher E. Wilmer*[1, 4]

[1]Department of Chemical & Petroleum Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania 15261, United States

[2]Department of Chemistry, University of California, Berkeley, Berkeley, California 94720, United States

[3]Department of Mechanical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, United States

[4]Department of Electrical & Computer Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania 15261, Unites States

Included Sections

1. Thermal conductivity as a function of correlation time plots for correlated defect nanoregions.

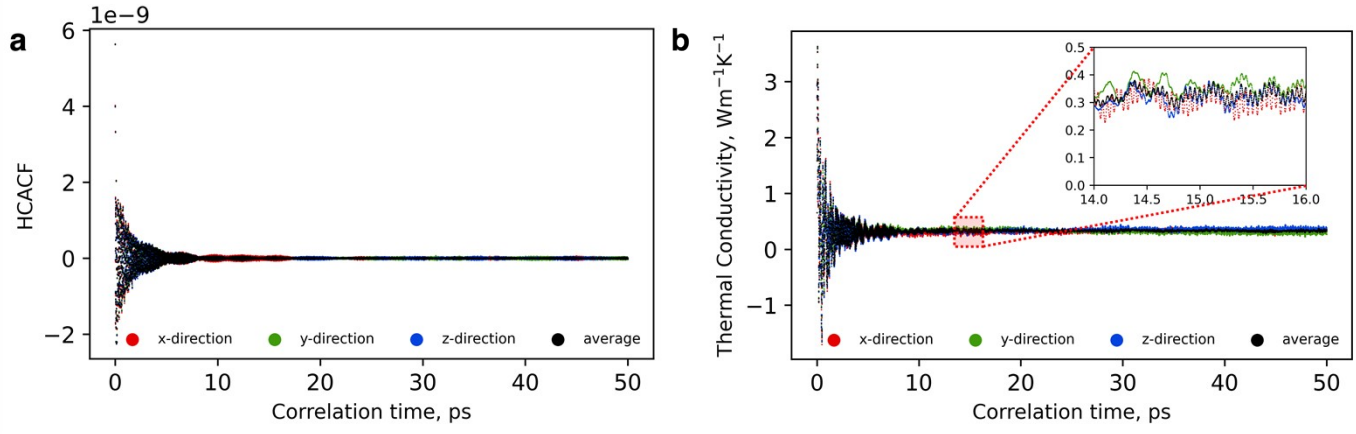

Figure S1. The HCACF **(a)** and thermal conductivity **(b)** plotted as a function of correlation time for pristine UiO-66 (3x3x3 supercells).

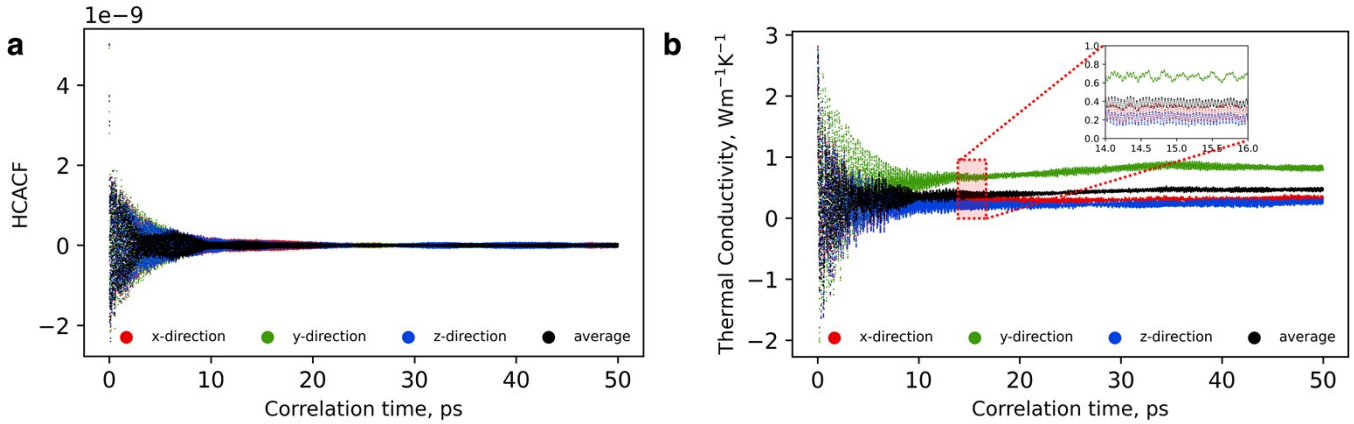

Figure S2. The HCACF **(a)** and thermal conductivity **(b)** plotted as a function of correlation time for missing linker correlated defect nanoregions (**bcu** topology).

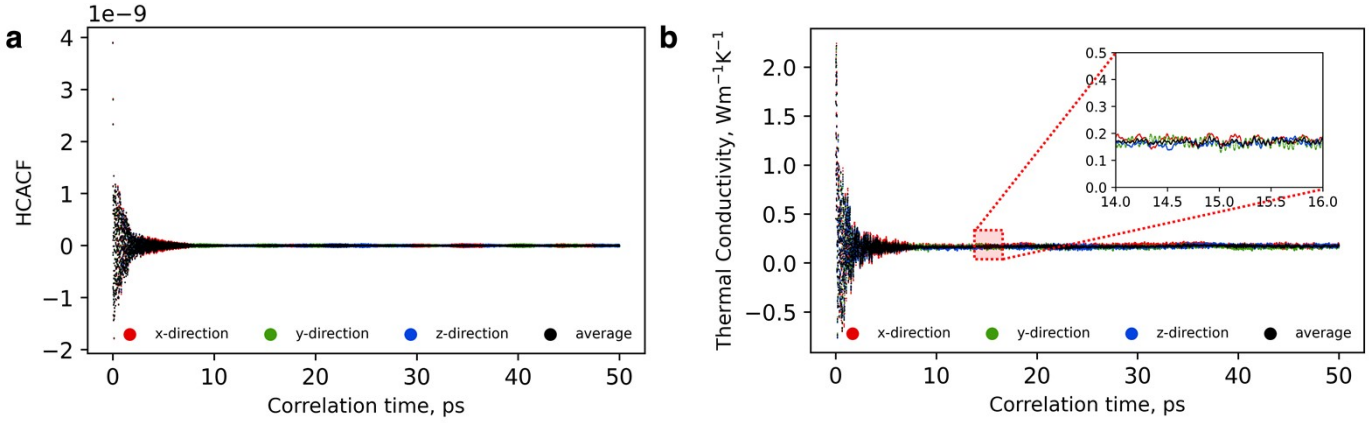

Figure S3. The HCACF **(a)** and thermal conductivity **(b)** plotted as a function of correlation time for missing cluster correlated defect nanoregions (**reo** topology).

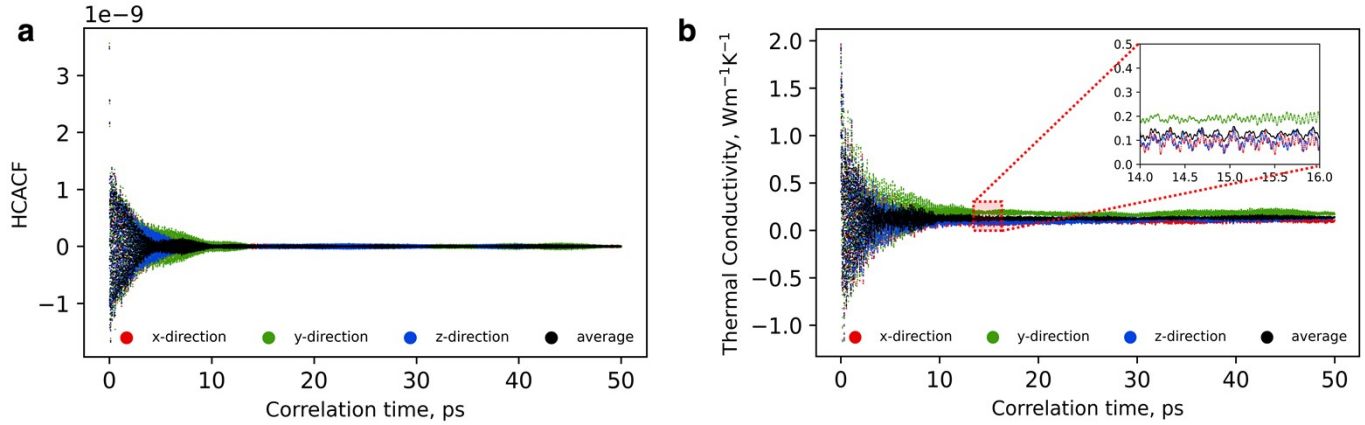

Figure S4. The HCACF **(a)** and thermal conductivity **(b)** plotted as a function of correlation time for missing cluster correlated defect nanoregions (**scu** topology).

2. Relationship between thermal conductivity and defect concentration

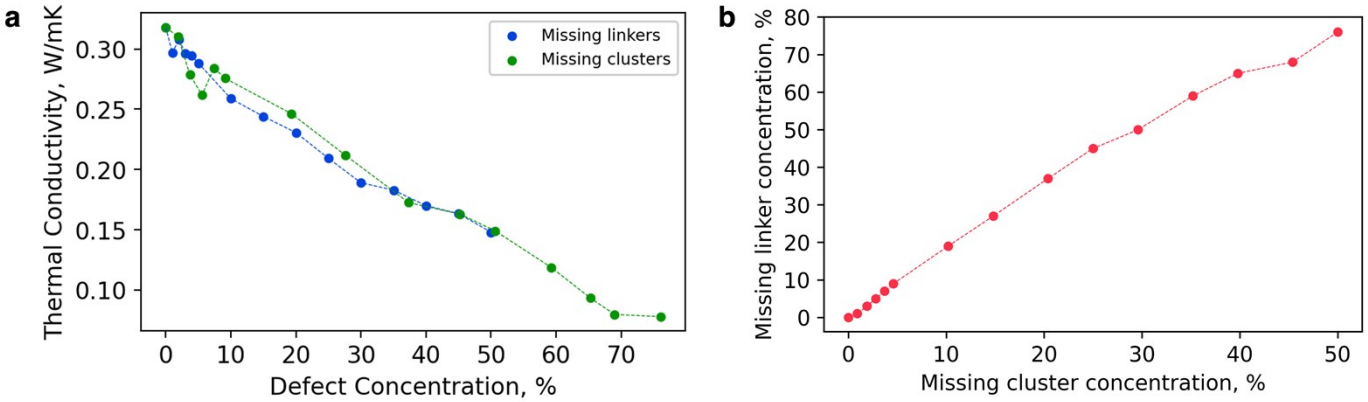

Figure S5. (a) Relationship between thermal conductivity and defect concentration, plotted against missing linker defect concentration as the x-axis, for UiO-66 with randomly incorporated missing linker and missing cluster defects (one replicate only). **(b)** Corresponding missing linker concentration as a function of missing cluster concentration for randomly incorporated missing cluster defects.

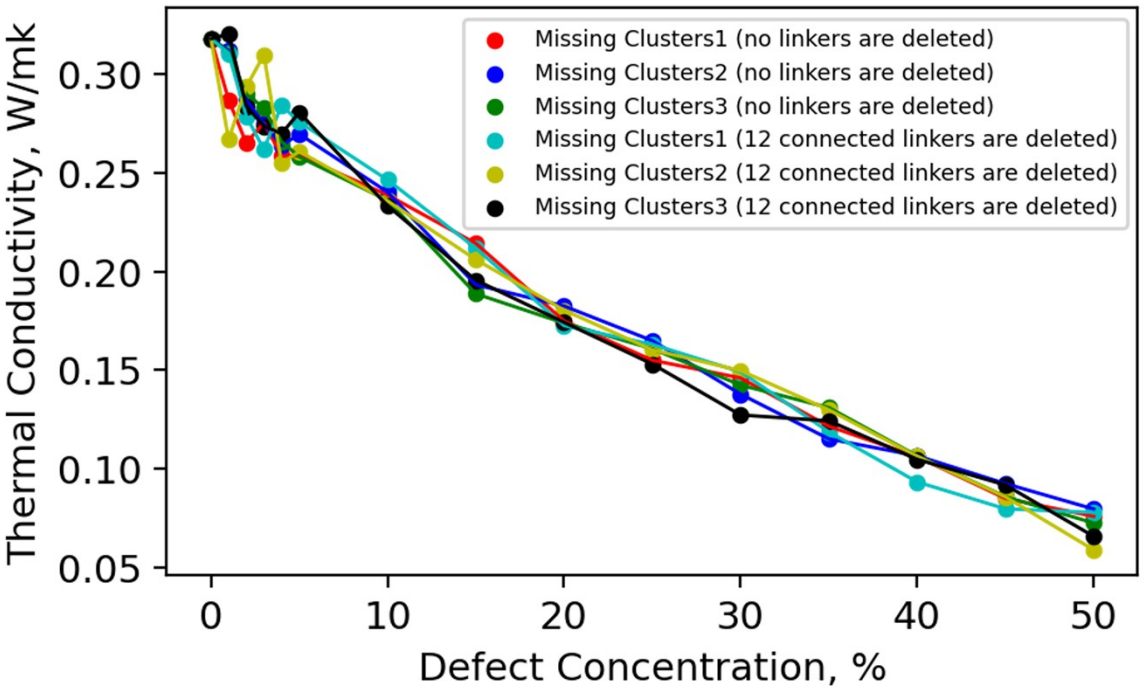

Figure S6. Relationship between thermal conductivity and randomly incorporated missing cluster defect concentrations, considering the deletion and non-deletion of all 12 linkers connected to the node.

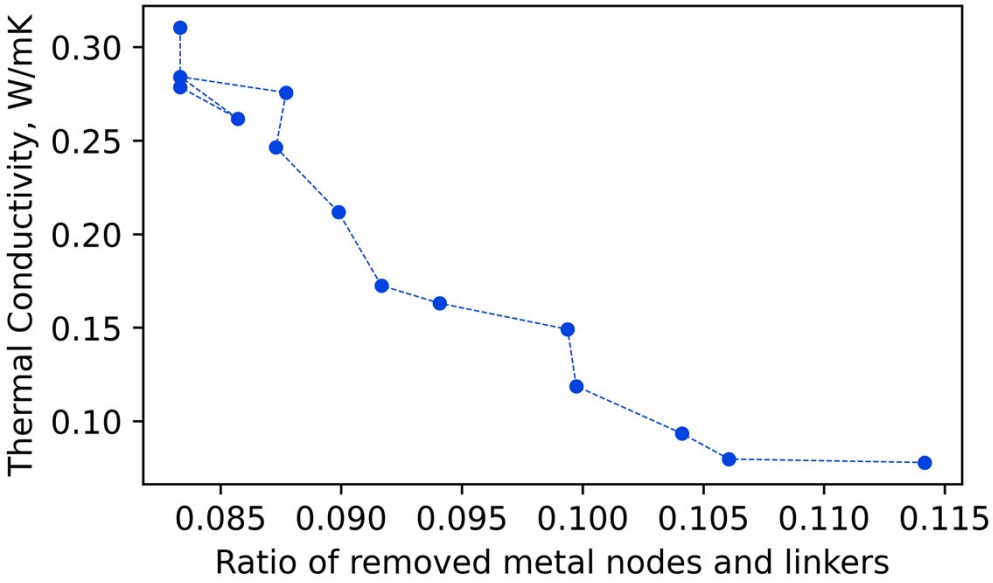

Figure S7. Relationship between thermal conductivity and the ratio of removed metal nodes to linkers for defective UiO-66 with randomly incorporated missing cluster defects.

3. Relationship between mass density and defect concentration.

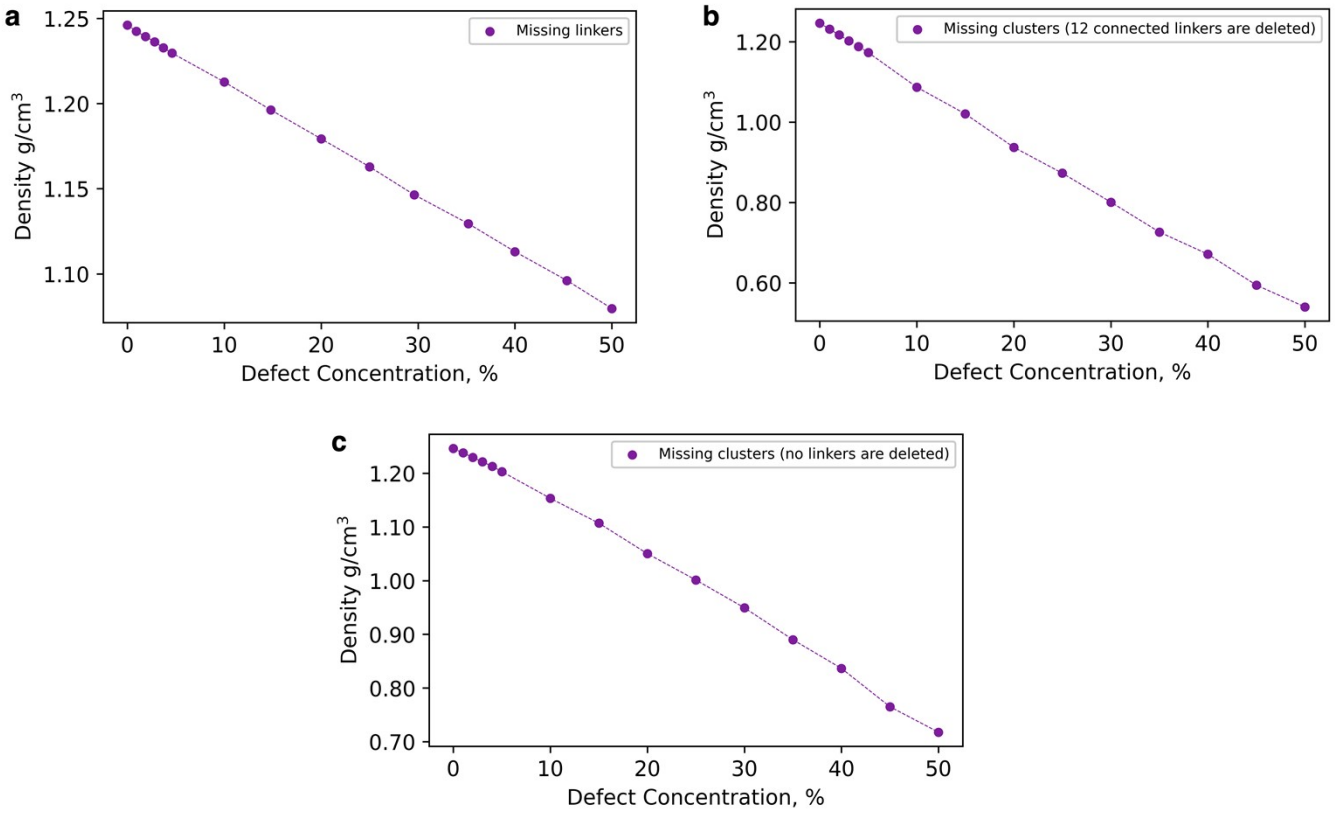

Figure S8. Relationship between mass density and defect concentration for UiO-66 with randomly distributed defects: **(a)** missing linker defects; **(b)** missing cluster defects where all connected 12 linkers are deleted; **(c)** missing cluster defects where no linkers are deleted.

4. Phonon dispersion relations.

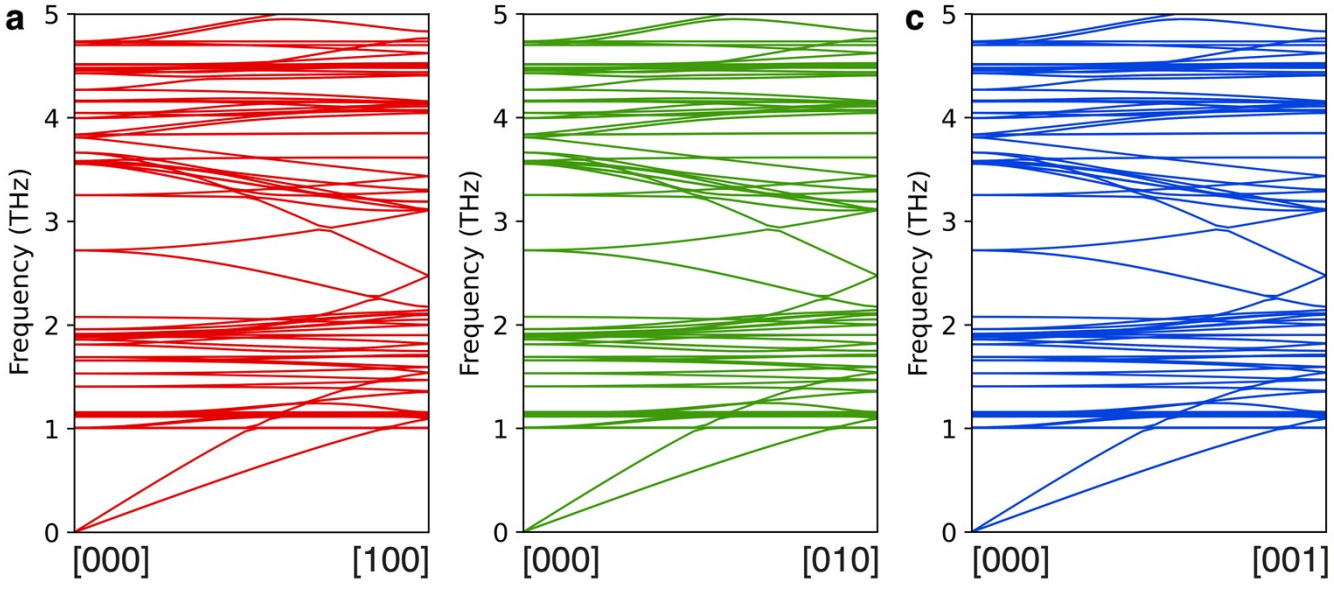

Figure S9. Phonon dispersion curves for pristine UiO-66.

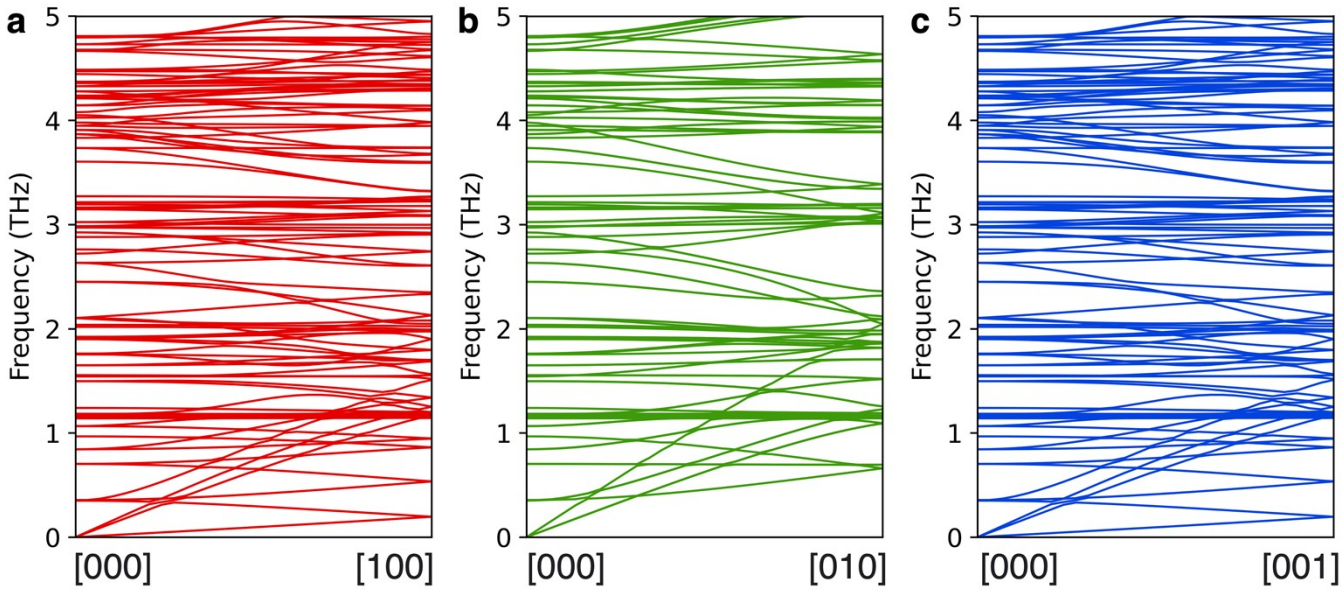

Figure S10. Phonon dispersion curves for defective UiO-66 with correlated missing linker defects (**bcu**).

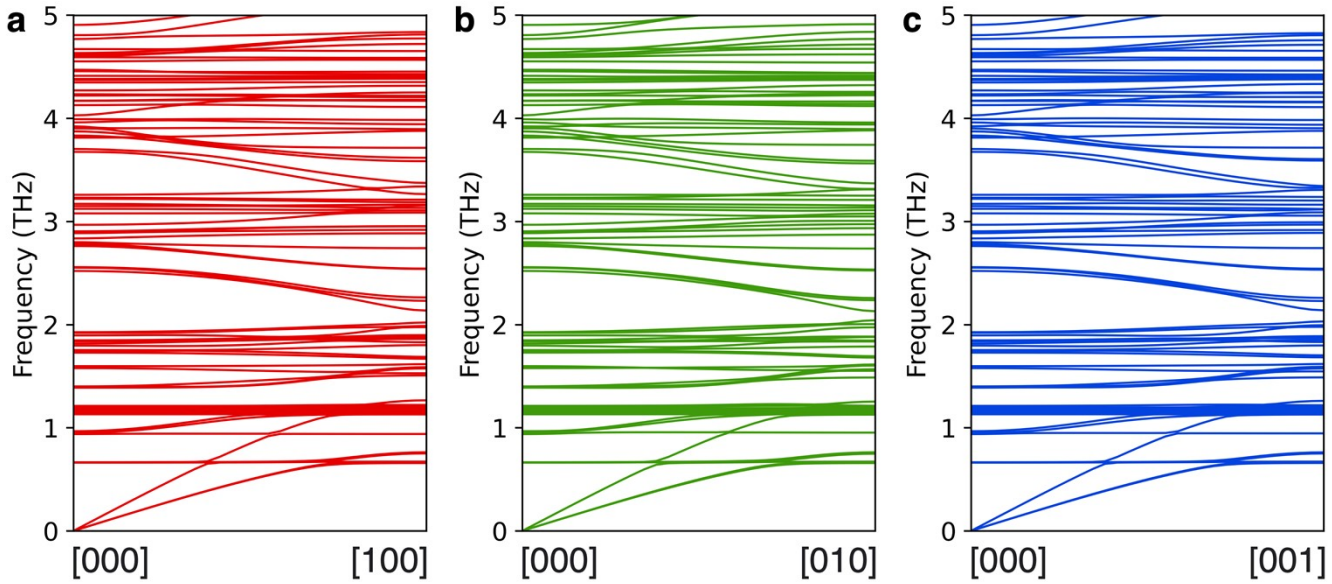

Figure S11. Phonon dispersion curves for defective UiO-66 with correlated missing cluster defects (**reo**).

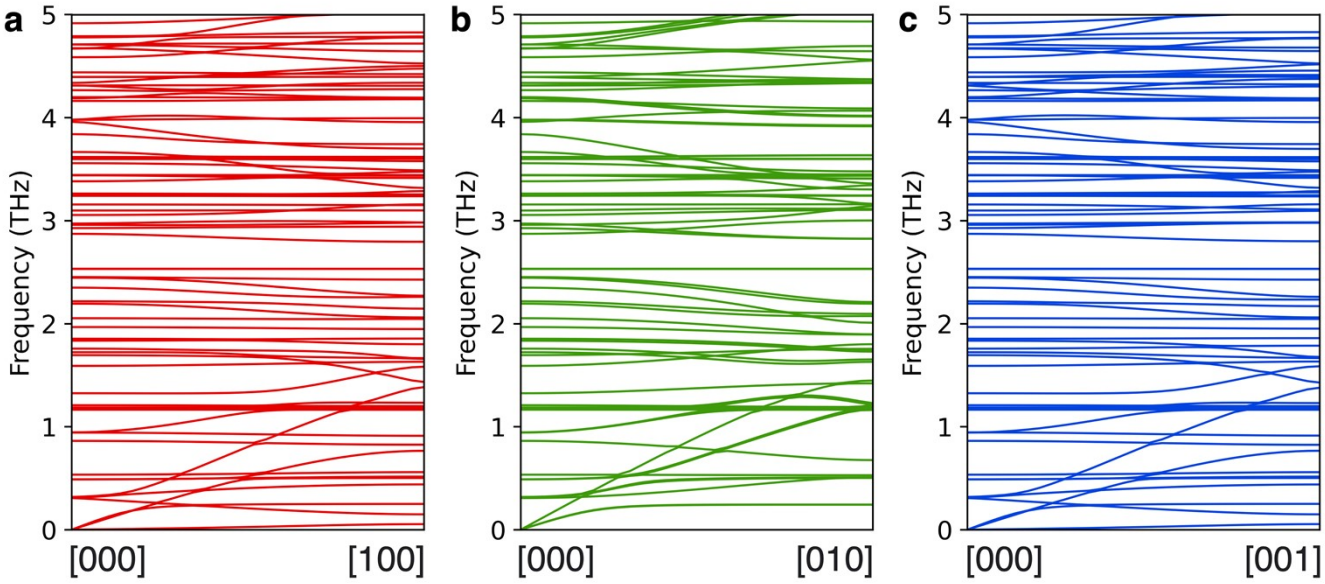

Figure S12. Phonon dispersion curves for defective UiO-66 with correlated missing cluster defects (**scu**).

5. Phonon density of states (DOS).

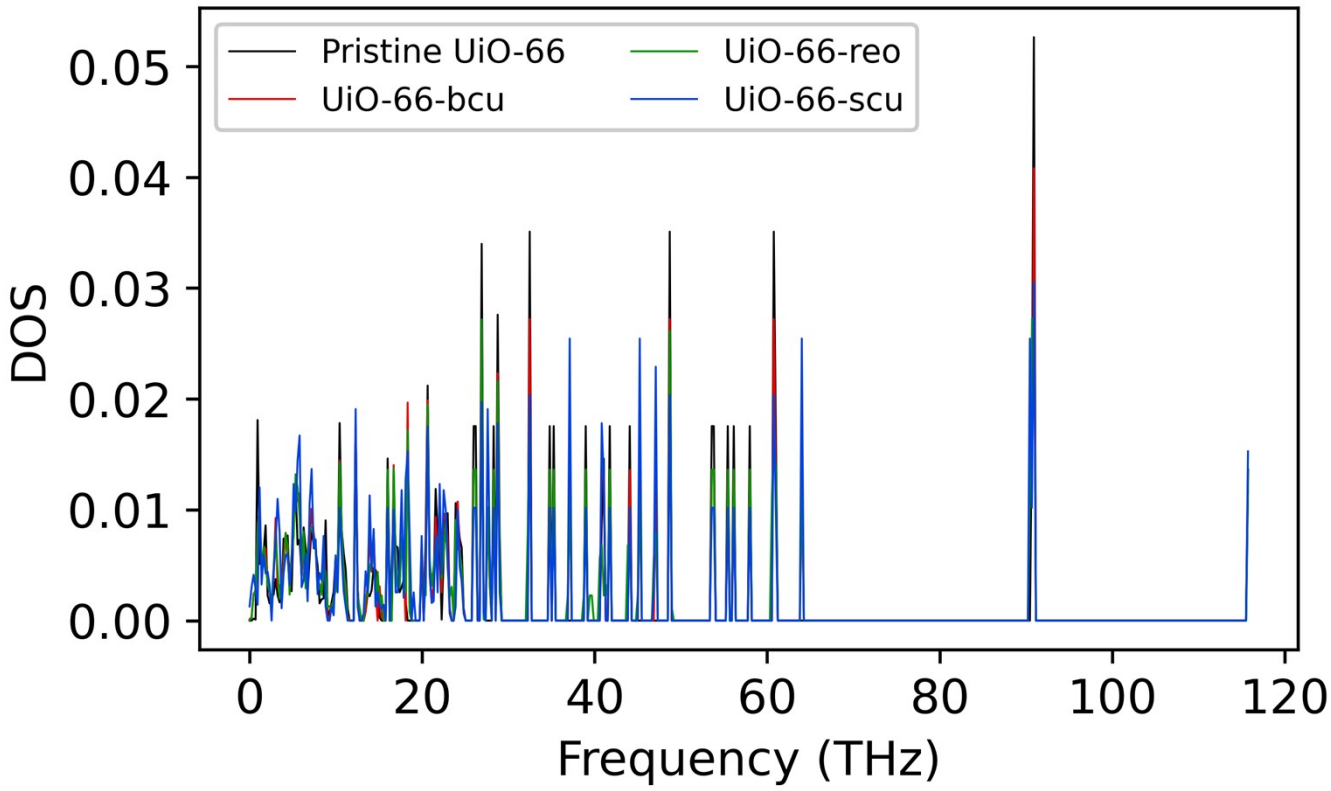

Figure S13. Vibrational density of states (DOS) for pristine UiO-66 and defective UiO-66 with correlated defects (**bcu**, **reo**, and **scu**).