Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Performance of GFN1-xTB for periodic optimization of Metal Organic Frameworks

Maryam Nurhuda [a], Carole C. Perry [a], Matthew A. Addicoat[a]*

[a] *School of Science and Technology, Nottingham Trent University, Clifton Lane, Nottingham NG11 8NS*

Supporting Information:

1. Optimised geometry of Cu, Ni, Zn- based M_2O building units and RMSD of bond length M-M and M-O.
2. Optimised geometry of In, Fe, Al- based M_3O building units and RMSD of bond length M-M and M-O.
3. Volumetric surface area of structures with preoptimised VSA in between 800-1200 m^2/cm^3 .
4. Method to identify structures with huge nodes and thin linker and example structures.

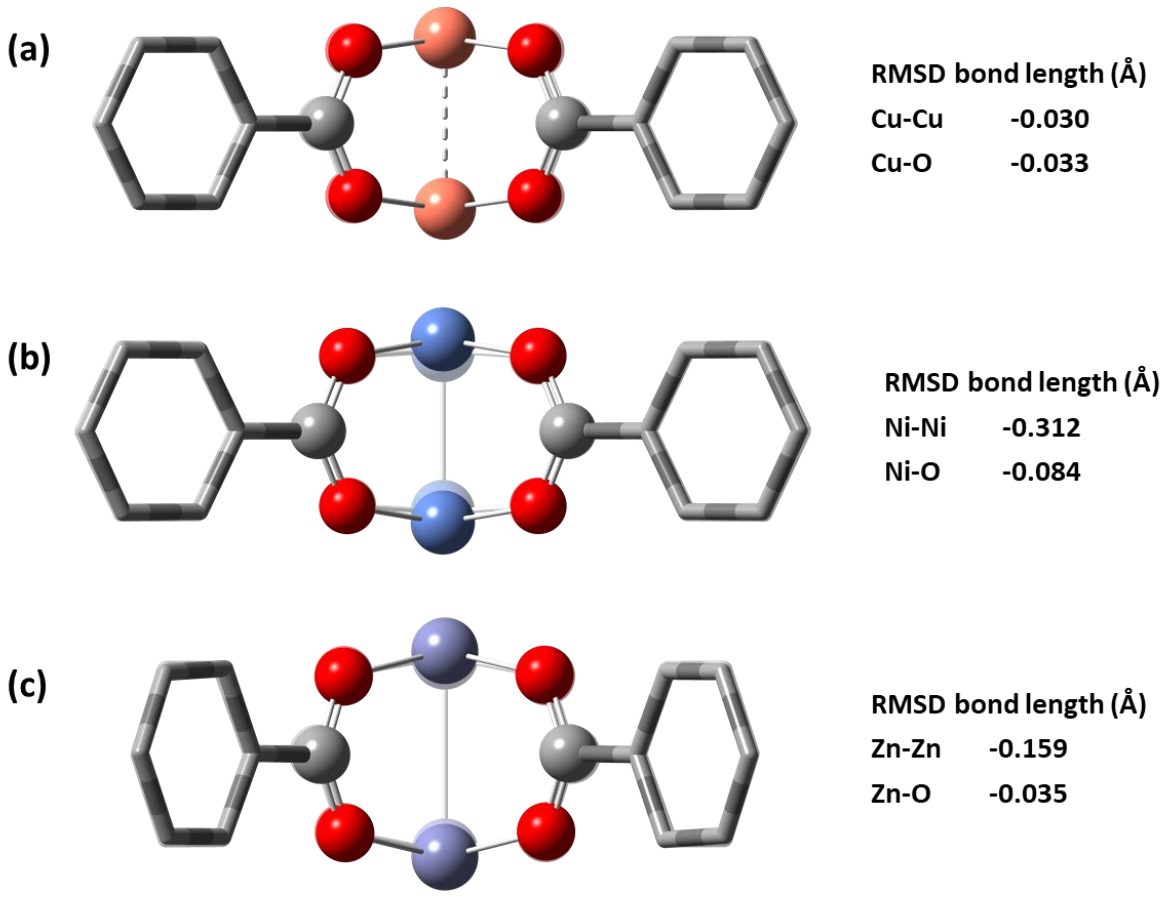

Figure S1. M_2O Paddlewheel (a) Cu_2O Refcode FIQCEN (b) Ni_2O Refcode EZOFEF (c) Zn_2O Refcode FUTKEL. Crystal structure is represented by opaque and optimised structures are shown partly transparent.

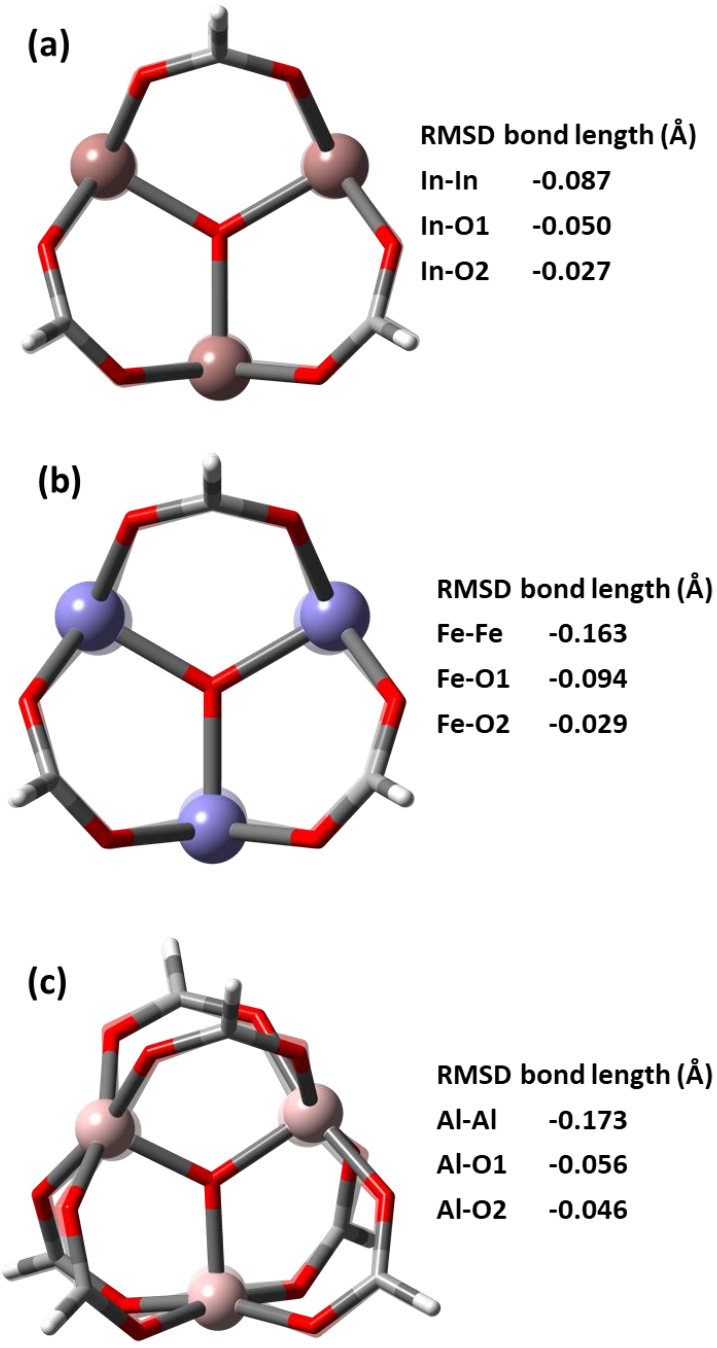

Figure S2. Trimeric oxo-centred M_3O (a) In_2O refcode FIFGIM (b) Fe_2O refcode HAKSIY (c) Al_2O refcode JALCAD. Crystal structure is represented by opaque and optimised structures are shown partly transparent

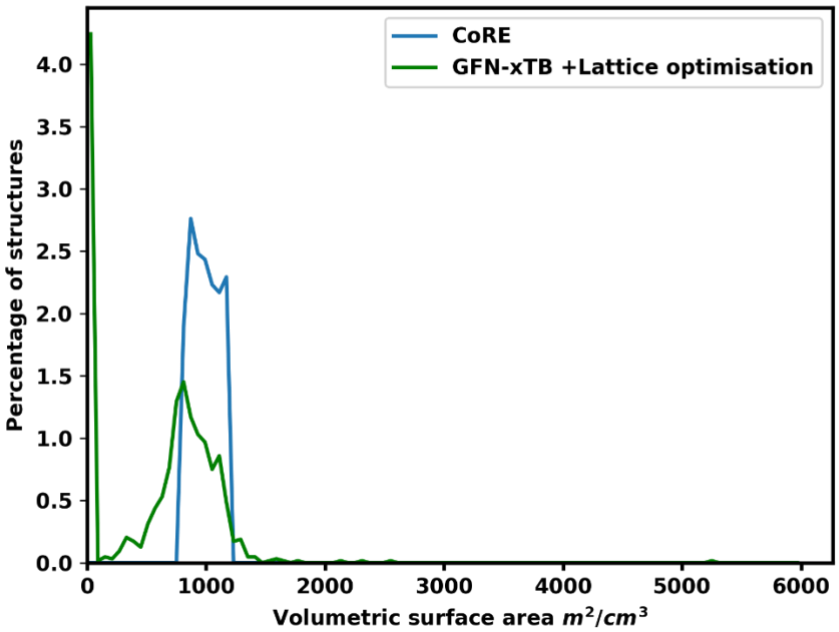

Figure S3. Volumetric accessible surface areas of CoRE structures with preoptimised VSA in between 800-1200 m^2/cm^3

S4. Method to identify structures with linkers that are relatively small compared to the size of metal node.

The structures which we described as ***metalvsorganic*** (in CoREdatabase.xlxs) are excluded from the dataset, the organic linker is too thin to support the metal nodes which makes the structure collapse during the optimisation. The method that is used to identify the structures is the percentage of organic atoms (excluding O and H) less than 20% for structure with total number of atom in between 150-250 or the percentage of organic atoms (excluding O and H) less than 33% for structure with total number of atom more than 250.

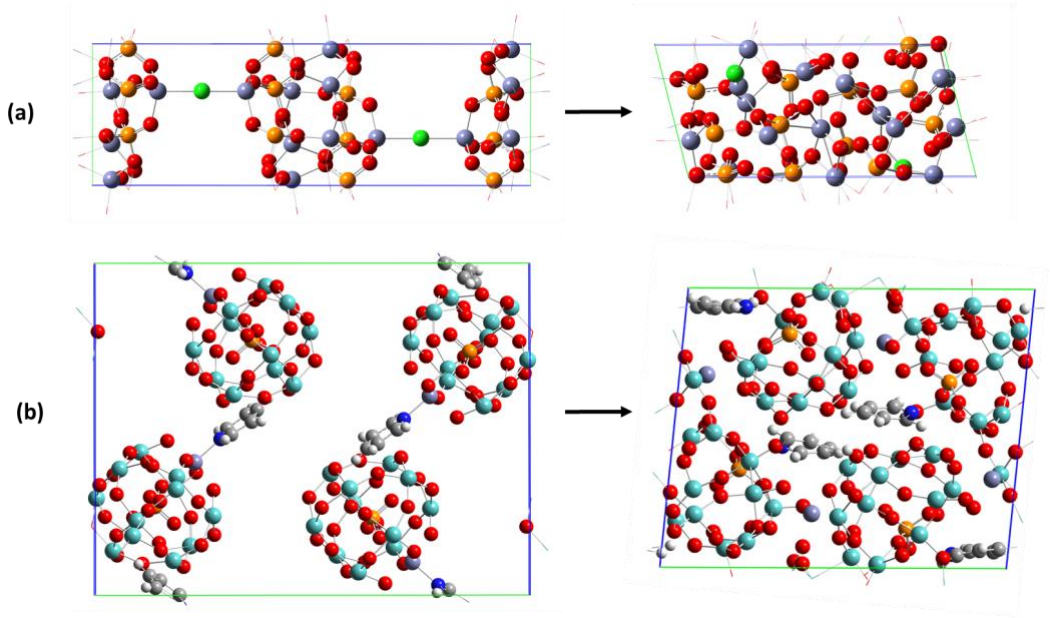

Figure S4. Structures with thin linkers compared to size of metal node. Refcode (a) ACUBAB_clean (b) C6DT02320G_c6dt02320g2_clean