

Pyrene-based metal organic frameworks

Interactive visualization of the crystal structures of pyrene-based MOFs, as an extension of Table 1 of the review "Pyrene-based metal organic frameworks: From synthesis to applications". The crystal structures have been manually curated to fix partial occupancy and remove solvent, and, if charge neutral, submitted to DFT cell optimization following the CURATED protocol described in 10.1021/acscentsci.9b00619. In this DISCOVER page the reader can browse through the list of MOFs, lend to the reference paper, visualize the crystal structures, and visualize their properties in a scatter plot. For the structures that are charges or failed the DFT optimization the properties and the unit cell of the original (manually cleaned) structure are shown.