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DFT comparison of MOFs containing BCP cages and covalent-organic frameworks. By using density functional theory (DFT), single-component homonuclear, 4-connected boron-centered (4CC) cage clusters B(4)(2+) or B(4)(3+) and their 2D and 3D boron-based coordination polymers are evaluated in terms of their stability, electronic structure, and reactivity. The presented results show that there is a limit to the maximum coordination number for each of the homonuclear boron clusters B(4)(2+) and B(4)(3+), with a maximum of four. The search for 3D coordination polymers containing the boron clusters B(4)(2+) leads to boron-based frameworks with up to three additional B(4)(2+) cages per unit cell. Such a 3D coordination polymer, the famous MIL-53, is constructed from hexagonally coordinated B(4)(2+) cages, with the resulting inorganic skeleton having a honeycomb topology. Searching for MOF structures containing hexagonally coordinated B(4)(3+) cages leads to 4CC heteronuclear boron-based clusters with up to 12 B(4)(3+) centers in the unit cell, the so-called MIL-47 and MIL-48. Under electron-deficient conditions, 4CC clusters can be incorporated in covalent-organic frameworks (COFs) with pyrimidines. The COF materials are investigated by DFT and experimental methods and are compared in terms of stability, electronic structure, and pore size. The comparison shows that the formation energy of MIL-48 is nearly twice as large as that of the COF with pyrimidine, suggesting that the COF is significantly more stable.

Q: Group Matplotlib figure by y tick values I am using matplotlib to generate a figure in which the y ticks are determined by a function (an unknown parameter) that I would like to determine experimentally, rather than changing the figure by hand. I can do this fine for the x tick labels. Is it possible to do the same

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