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Thermodynamic Stability Analysis of Metal Organic Frameworks

YEJIN KIM, Taft School, RICHARD KYUNG, Choice Research Group — Metal-Organic frameworks bear a huge potential for various developments in many different fields of science. This study seeks to study the stability and dynamics of different types of MOFs in various conditions, such as with different metal joints or linkers with different functional groups. In a more general sense, this research aims to contribute to the materialization of MOFs full usage in green energy and eco-friendly technologies. This research performs thermodynamic and stereo-chemical analysis of Metal Organic Frameworks. In this paper, Density Functional Theory (DFT), a computational chemistry, has been employed to figure out the stability and thermodynamics of different structures of MOFs, and to model the electron properties of the compound. With Avogadro and Chemcraft, programs that allow users to draw and estimate enthalpy for a compound, and Matlab which gives numerical estimate of electric potential between the capacitors, this research demonstrates the optimized geometry energy levels and fully determines the theoretical values of the structures atomic properties.

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None

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