Abstract Submitted
for the MAS20 Meeting of
The American Physical Society

Study on the Metal-organic Frameworks for Sustainable Energy Using Various Metals and Linkers DAVID JAEMIN CHOUNG, Kimball Union Academy — 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 including UIO-66 in various conditions, such as with different metal joints or linkers with different functional groups. 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 molecular editing programs that allow users to draw and estimate optimized energy and electrostatic potential maps for a compound, this research demonstrates the optimized geometry energy levels and fully determines the theoretical values of the structures atomic properties. The research focuses on increasing capacity of batteries using MOF particles as dielectrics, differing the structure of capacitors, and various combinations of inorganic metal joints and organic carbon links in order to increase the maximum capacity of batteries that can store more energy with better efficiency. Computational chemistry such as Avogadro and ChemCraft has been employed to figure out the stability and capacity of the MOF particles.

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Date submitted: 02 Nov 2020 Electronic form version 1.4