# Study on the Optoelectronic Behavior of Zr Based MOFs Using Computational Simulations

Richard Kyung
*CRG-NJ*
*Cresskill, NJ, USA*
richardkyung@choicerg.com

Woong Jae Baek
*UIUC*
*Urbana, IL, USA*
wbaek3@illinois.edu

Andrew Kim
*Cooper Union*
*New York, NY, USA*
kim70@cooper.edu

***Abstract* —The research focuses on studying the behavior of MOFs(Metal Organic Frameworks) used in optoelectronic device. By differing the structure of particles, chemical and physical behaviors of various combinations of inorganic metal joints and organic carbon links were studied in order to efficiency of the optoelectronic device. Computational physics and chemistry such as Gaussian and ChemCraft have been employed to figure out the stability and efficiency of the MOF particles. Avogadro was used to optimize the movement of elements and find potential maps within particles. Thermodynamic stability, VSEPR principles and modeling techniques are also used to calculate optimization energy of the various linkers and joints of the MOFs. Research shows the high electro potential and optimized enthalpy in Zr based MOFs are observed.**

***Keywords— MOFs, Photocatalytic Activity, Optoelectronic device, Organic joints, Photoluminescence, Optimization energy***

## I. INTRODUCTION

Advancements in micro technology resolve previously-common technological problems in electro-chemical and electro-physics systems. Developing technology allows a significant reduction in the size of optoelectronic device systems. High voltage can be sent through a smaller optoelectronic device system, and across a optoelectronic device, which remains to have a high photocatalytic activity and high photoluminescence.[1] Using the ideal geometry and dimension of a MOF system, computational solutions are attained, which is useful in the comparison between experimental results and virtual simulations.

The study considers the electrodes or plates exhibiting the effect of the photocatalytic activity and photoluminescence in the single and multi-layered optoelectronic device system. A complete set of known dimensions and insulating characteristics allows the system to be determined. Then, the relationship between electric and thermodynamic properties of the materials are computationally calculated.

The relatively recent discovery of metal organic frameworks, porous materials mainly composed of carbon linkers and metallic parts, have come to fore for its ability to store and capture desired elements in itself. As research in the field of metal organic framework advances, the possibility of utilizing MOFs in batteries to increase capacitance is becoming actualized. In a world where we lack energy and need more efficient sources of storage, such micro particles will enable us to enhance the amount of electronic storage and utilize in the following decades. Through this research, we aim to discover whether MOF particles are replaceable as dielectrics between optoelectronic device and how efficient they can be. [2]

Though largely unexplored, MOFs can also be integrated into electrochemical optoelectronic device, which are high power density energy storage devices. In the past, zeolites or porous carbon materials, such as activated carbons, have been used in commercial optoelectronic device that function by storing charge on electrochemical layers. Now, nMOF driven optoelectronic device in which films composed of nMOFs and other medium are placed on a layer soaked by a solution of an electrolyte, outperform the above materials because of their high porosity and structural versatility. Such development has persuaded many scientists to believe that MOFs may hold a key to the breakthrough in renewable and sustainable energy development. [3]

## II. PROCEDURES AND METHODS

To build efficient nMOF driven optoelectronic device, all experimental devices/parts were arranged and placed properly in this experiment. Specifically, focus was placed on placing all films made from nMOFs doped with graphene on both sides of a separator membrane and soaking the construct in the solution of an electrolyte. Information on the detailed procedures for synthetic preparation and analysis of nMOFs including their characterization data was collected for this research. [5]

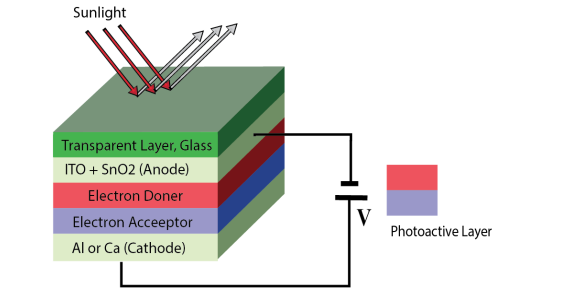
Our construct for incorporating nanocrystals of MOFs into optoelectronic device is based on a coin-type device composed of films made from nMOFs doped with graphene. The films are placed on both side of a separator membrane and soaked by a solution of an electrolyte. It is expected that by charging the device, the positive and negative ions of the electrolyte move in opposite directions through the separator and into the MOF pores. During discharge, the ions migrate out of the pores and the electrons flow out of the device. MOFs would perform well in this context because of their high porosity and openness of their structure, which should give high capacity for storage of ions and robust cycling of ions within the cell, respectively.

The pore environment produced by multiple functionalities clearly influences the capacitance in the nMTV-MOF-5 series. Members of a new class of chemically and thermally stable MOFs based on zirconium (IV) show progressively better performance as pore diameter decreased.

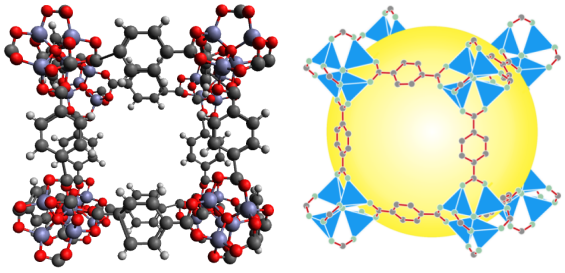
Density Functional Theory (DFT), a computational and quantum chemistry, is used in order to model the electron properties of the MOFs compounds in the optoelectronic device. Avogadro is an open-source molecular editing program with an auto-optimization feature that determines the theoretical values of the structure's atomic properties. It allows users to build virtually any molecule with the optimized geometry according to various force field options.

## III. APPLICATIONS

The optoelectronic device employing MOFs represent an important class of energy transfer or light emitting diodes(LEDs) because of their remarkably high power densities. Porous carbon materials such as activated carbon are commercial product that operate by storing charge on electrochemical layers. This is in contrast to the storage of charge by redox reactions as exemplified by metal oxide pseudo-capacitors. Each of these classes optoelectronic device has strengths and weaknesses: carbon-based materials operate at very high charge/discharge rate with long lifecycle but have low capacitance, while metal oxide materials have high capacitance but their redox reactions lead to low lifecycle. [6]




(a) p-n junction-electron donor/acceptor



(b) MOF constructed usig Avogadro (c) MOF 5 model

Fig. 1. Constructured structure of MOF 5 as an electron donor

Also, to find characteristics of longitudinal vibration of a long uniform rod of length *l* and mass/length h, data were defined as:

### *A. nUIO and nMOF*

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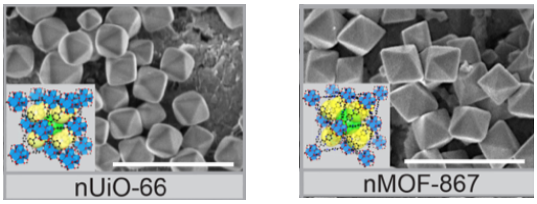


Fig. 2. Uniform structure of MOF particles

### *B. Analysis of MOF Particle – Computational*

As complexity increases, the optimized energy increases as well, albeit with increased variation within cluster.

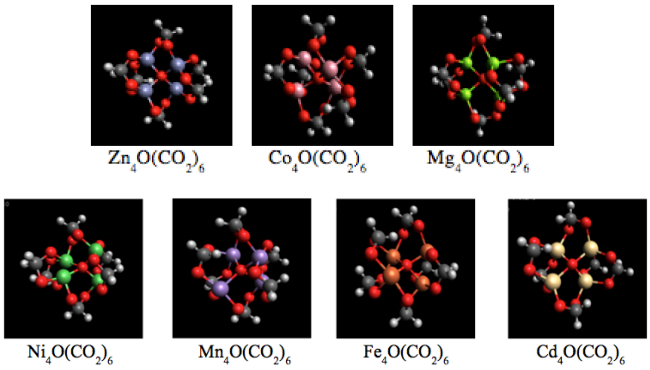


Fig. 2. Various joints and 7 metals – Opt. E computed by Avogadro

TABLE I. OPTIMIZED ENERGY OF VARIOUS JOINTS AND 7 METALS

| Compounds | Molecular Formula | Molecular Weights (g/mol) | Optimization Energy (kJ/mol) |
|---|---|---|---|
| $M_1O(CO_2)_6$ | $Zn_4O(CO_2)_6$ | 553.672 | 324.858 |
| $M_2O(CO_2)_6$ | $Co_4O(CO_2)_6$ | 527.884 | 1,325.666 |
| $M_3O(CO_2)_6$ | $Mg_4O(CO_2)_6$ | 389.372 | 372.661 |
| $M_4O(CO_2)_6$ | $Ni_4O(CO_2)_6$ | 526.925 | 1,512.325 |
| $M_5O(CO_2)_6$ | $Mn_4O(CO_2)_6$ | 511.904 | 1,143.882 |
| $M_6O(CO_2)_6$ | $Fe_4O(CO_2)_6$ | 515.532 | 1,175.643 |
| $M_7O(CO_2)_6$ | $Cd_4O(CO_2)_6$ | 741.796 | 330.047 |

With the organic linkers and metal joints modelled above, MOF particles are able to contain much gas particles and electrons through remarkable increase in surface area. A revolutionary in the field of Metal Organic Frameworks, Professor Omar Yaghi at the University of California, Berkeley, discovered the MOF-5 particles with his group of researchers who made a remarkable achievement by effectively increasing the surface area of these nanoparticles.

TABLE II. OPTIMIZED ENERGY OF VARIOUS ELEMENTS

| Compounds | Molecular Weights (g/mol) | Optimized Energy (kJ/mol) | Electro Potential (V) |
|---|---|---|---|
| Cd | 741.796 | 1017.431 | 0.000 |
| Zr | 657.048 | 12.466 | 0.000 |
| Ta | 1015.943 | 18.679 | 0.000 |
| Nb | 663.777 | 15.088 | 0.000 |

The photocatalytic activity of the elements in the Table II turned out to be zero before they are used in the MOF as components.

### *C. Effect of Metals*

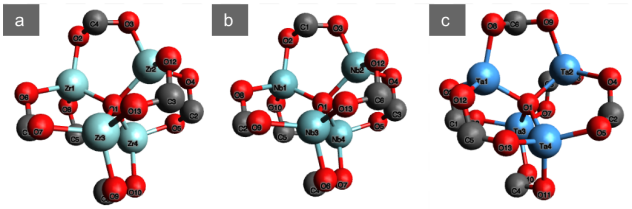


Fig. 3. Optimized shapes of the metals and joint complex ((a)Zr, (b)Nb, and (c)Ta)

### *D. Effect of Linkers*

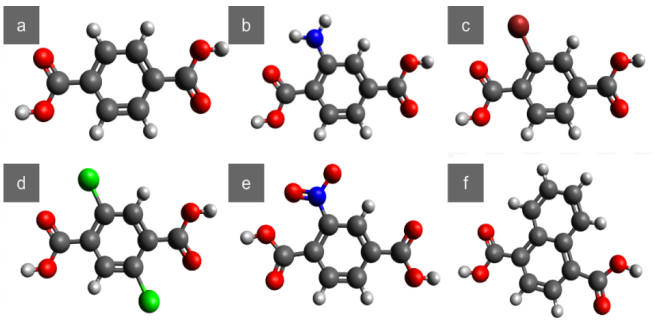


Fig. 4. Optimized shapes of the various linkers of MOFs

The photocatalytic activity of the clusters in the linkers in the Fig. 4 shows higher than that of each elements.

TABLE III. OPTIMIZED ENERGY OF VARIOUS FUNCTIONAL GROUPS

| Compounds | Molecular Formula | Molecular Weights (g/mol) | Optimized Energy (kJ/mol) | Electro Potential (V) |
|---|---|---|---|---|
| Terephthalic acid (a) | C8H6O4 | 166.13 | 72.91 | 0.000 |
| 2-aminoterephthalic acid (b) | C8H7N0O4 | 181.15 | 109.8 | 0.269 |
| 2-bromoterephthalic acid (c) | C8H5BrO4 | 245.03 | 90.34 | 0.888 |
| 2, 5-dichloro terephthalic acid (d) | C8H4Cl2O4 | 235.02 | 104.30 | 0.000 |
| functional group (e) | C8H6NO6 | 212.14 | 162.39 | 2.684 |
| naphthalene-1, 4-dicarboxylic acid | C12H8O4 | 216.19 | 205.88 | 0.243 |
| (f) | | | | |

## IV. DISCUSSIONS AND CONCLUSIONS

Various porous metal-organic frameworks representing a diversity of structure types and metrics, sizes and functionalities of pores were targeted for their computational analysis in nanocrystalline form, study of their performance, and properties as optoelectronic device. It is significant that the energy profiles of these nMOFs change differently and follow the general behavior expected in VSEPR theory.

This research investigated the functionality and stability of MOF molecules at the same time, finding better chemical compounds with less optimization energy. The more functionality there is, the more heat(enthalpy) it can give off, meaning that it needs more effort to stabilize the compound. We not only want complexity having more porosity, but also stability and efficiency. There is always a trade-off between stability and functionality.

The differences are the details of the electrochemical behaviors of nMOF. Perhaps their diverse structural and functional attributes are directly involved in electrochemical properties and depend on their chemical nature and structures. nMOF, the future breakthrough for the study of electrical and electrocatalytic medium in the optoelectronic device, and other applications of MOFs will need to find a right balance between stability and complexity based on the computational data.

Future work should focus on deciphering the specific impacts of various MOF structures on the optimization energy.

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