<u>Nanoengineering of Metal Organic Frameworks for Applications in CO_2 Capture, Drug Delivery, and Electronic Devices</u>

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Metal organic frameworks (MOFs), an emerging class of crystalline nanoporous materials, have recently caught attention for their unique properties such as high surface area, large pore volume, high uniform and permanent porosity, and ease of chemical tenability to introduce additional physical, chemical, or electrical properties. MOFs constructed from inorganic and organic pieces: metal ions and organic ligands, which play the role of linking metal nodes, respectively. Chemical versatility comes from the high variety of organic ligands (e.g. carboxylates, phosphonates) and metal centers (e.g. transition metals) available. Here, synthesis and characterization of MOFs for different applications, such as carbon dioxide capture, electroconducting materials, and drug delivery will be studied.

Currently, one of the heightened global concerns is increasing CO_2 concentration which is argued to be a factor in rising global temperature and climate change.[4] Carbon capture and storage technologies show promise in this field, with research currently focused on large CO_2 emissions sources such as coal fired power plants. Competitive CO_2 capture capacities were obtained with MOFs as adsorbents at the CO_2 partial pressures expected in post combustion flue gas. However, important considerations such as the presence of moisture (5-7% by volume in the flue gas) and material regenerability requirements should be accounted for when designing an efficient CO_2 adsorbent. MOFs are promising materials in this field since they can be modified to accommodate some of the requirements. In this work, pore surface modifications with functional groups have been shown to improve material stability under humid environment. The MOF of the study was magnesium dioxybenzenedicarboxylate (Mg/DOBDC) and it was functionalized with ethylenediamine groups. Characterization and CO_2 capture tests were performed and results were compared for both original Mg/DOBDC and functionalized Mg/DOBDC before and after exposure to humid conditions.

The second aim of this research is to synthesize a biodegradable MOF for future use in drug delivery. Proposed solution is to synthesize MOF material based on biomolecules already present in human body or naturally occurring, such as nucleobases, amino acids, and small biomolecules. Biomolecules are very diverse, can exhibit many metal-coordination sites, and can lead to biocompatible non-toxic materials. One of the first attempts will be to use nucleobase, such as guanine or adenine along with any of the small biomolecule (e.g. tartaric acid) for increased dimensionality and metals such as Zn or Mg, which are already present in the human body and could be a safe choice.

The third aim of this research is to synthesize electroconductive MOF material. There are currently only few conductive coordination networks reported. The proposed route is to use organic dye molecules currently used in dye sensitized solar cells as an organic linker molecule and Cu as a metal source. One such combination was reported in the literature and it is believed similar approach can lead to a conductive framework, due to the known light harvesting and transporting properties of organic dyes. Cu ion possesses high coordination number (4-6), which can lead to various structures. Electro conductive coordination frameworks can be useful in nanoscale electronic applications.