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MODELING FOR THE DESIGN OF ELECTROCHEMICAL ENERGY STORAGE MATERIALS

Takara Everest Truong (Roseanne Warren)
Department of Mechanical Engineering

The research objective of this project is to apply computational modeling to guide development of nano-porous materials for applications in electrochemical energy storage. By modeling chemical reactions and processes, we can sample various experimental outcomes before manufacturing, saving both time and resources. We chose to model the carbonization process of MOF-5 as it is a promising material for super capacitor electrodes due to its high porosity, Fig 1. To model the complex carbonization process of MOF-5, we approached the problem in three steps: 1) create a simple model based on nitrogen cubane decomposition and validate it with literature results 2) modify the previous model to simulate a porous carbon structure and validate it with literature results 3) modify the porous carbon structure model with values from MOF-5 and validate with experimental results.

For the model, we used a Monte-Carlo based simulation with a Reactive State Summation Potential (RSS) [1]. We validated our simplified model with literature results by comparing the decomposition of nitrogen cubane with Yunfeng Shi's [1]. Reported bond length of both models were identical at 1.1Å and atomization energy per atom of our model was -4.91eV compared to Shi's -4.90eV. Afterwards, we adapted the nitrogen cubane model to match the Mimetic Porous Carbon Model (MPCM) [2]. Once validation of the MPCM model is complete, the final stage towards modeling MOF-5 will be to add additional bond information between different atom pairs in the MOF-5 structure and to test against experimental results.

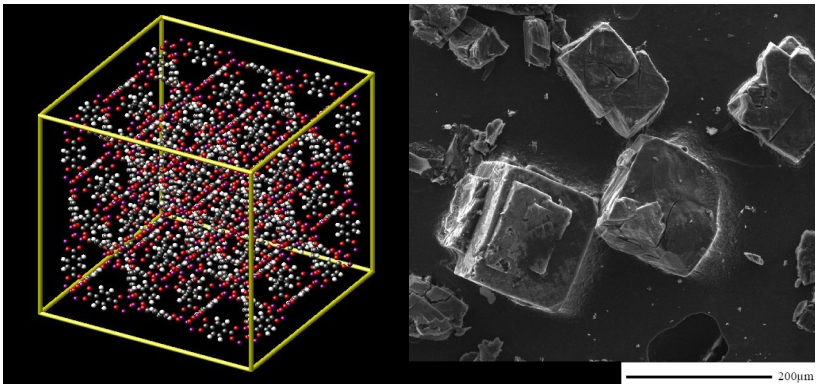

Fig. 1 MOF-5 Structure (Left), and SEM of MOF-5 (Right)

References:

[1] Y. Shi and D. W. Brenner, "Simulated thermal decomposition and detonation of nitrogen cubane by molecular dynamics," *The Journal of Chemical Physics,* vol. 127, no. 13, p. 134503, 2007/10/07 2007, doi: 10.1063/1.2779877.

[2] Y. Shi, "A mimetic porous carbon model by quench molecular dynamics simulation," *The Journal of Chemical Physics,* vol. 128, no. 23, p. 234707, 2008/06/21 2008, doi: 10.1063/1.2943645.