DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
SPRING 2022

DATE: WEDNESDAY, JANUARY 26, 2022

WEBEX:
https://njit.webex.com/njit/j.php?MTID=mdf236ae4dd5372831eabc5948adb47aa
Meeting number (access code): 2621 266 5639
Meeting password: CES

TIME: 1:00PM-2:20PM

GUEST SPEAKER

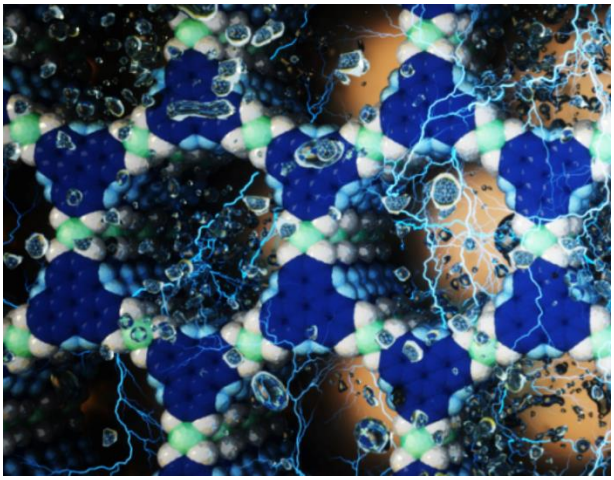
Dr. Farnaz Shakib
Assistant Professor
Department of Chemistry
NJIT
Newark, NJ

TOPIC

Structure-Functionality Relationships in Multifunctional 2D and 3D Metal-Organic Frameworks in Condensed Phase

ABSTRACT

The global ever-increasing demand for high-performance materials with complex functionality cannot be met without atomistic-level characterization and understanding the structure-functionality relationship. Such studies, however, are hindered by the large number of degrees of freedom as well as the complex and often quantum-mechanical nature of reactions in condensed phase. Novel computational platforms should be created which benefit from the efficiency of classical molecular dynamics but at the same time retain the accuracy of quantum-mechanical calculations. During this presentation, I will discuss our recent computational developments, as implemented in our open-source software package DL_POLY Quantum v1.0.[1], in the context of two families of nanoporous materials: two-dimensional (2D) π-stacked layered metal-organic frameworks (MOFs) and 3D zeolitic-imidazolate frameworks (ZIFs) [2-5]. I will show how theory can shed light on the responsive nature of 2D MOF architectures to external stimuli such as temperature, humidity, and photoexcitation. For the ZIF family, I will discuss two cases of (i) atomistic molecular dynamics simulations applied to large realistic nanoparticles in aqueous solution and (ii) the effects of incorporating nuclear quantum effects (NQEs) into the simulations using Feynman's path integral formalism [6]. Finally, I will elaborate on our future research path and how we are utilizing path integral formalism to incorporate NQEs into the non-adiabatic dynamics of charge transfer reactions in condensed phase.



References:

1) Momeni, M. R.; Shakib, F. A. *The DL_POLY Quantum molecular simulation package.* **2021**, Available from: https://github.com/mrmomeni/DL_POLY-Quantum-v1.0.
2) Shi, Y.; Momeni, M. R.; Chen, Y.-J.; Zhang, Z.; Shakib, F. A. *Chem. Mater.* **2020**, *32*, 9664.
3) Momeni, M. R.; Zhang, Z.; Dell'Angelo, D.; Shakib, F. A. *APL Mater.* **2021**, *9*, 051109.
4) Zhang, Z.; Dell'Angelo, D.; Momeni, M. R.; Shi, Y.; Shakib, F. A. *ACS Appl. Mater. Interfaces* **2021**, *13*, 25270.
5) Dell'Angelo, D.; Momeni, M. R.; Shaina, S.; Shakib, F. A. *J. Chem. Phys.* **2022**, in press, https://doi.org/10.1063/5.0076640.
6) Feynman, R. P. *Rev. Mod. Phys.* **1948**, *20*, 367.

Seminar Coordinator:
Dr. Genoa Warner – grw4@njit.edu
Dr. Amir Varkouhi - amir.k.varkouhi@njit.edu