

Wednesday, September 5 2018, 4:10-5:00PM, WEB 1230

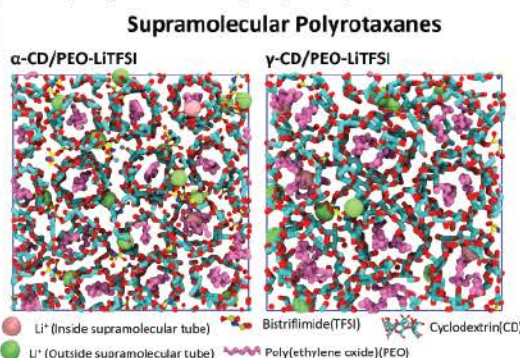
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Role of Molecular Dynamics Simulations in the Study of Energy-storage Materials

Molecular dynamics simulation, based on the representation of classical physics from quantum mechanics, is an established tool to understand molecular-scale phenomena of materials and chemical reactions [1]. In this presentation, I'll show how MD simulations can be applied in the study alkaline fuel cell membranes and electrolytes for lithium-ion batteries (LIBs) [2,3]. Knowing the beauty of materials at molecular scale helps us to obtain in-depth comprehension about structure-property relationship, non-trivial mechanistic correlation, and provides principles for the improvement of experiments. As a case study, this presentation will also show how experimental studies and MD simulations can work together to correct the previous misunderstanding about the Li^+ transport in LIBs electrolytes, self-assembled from supramolecular rotaxanes, and derive a systematic way to increase the conductivity of Li^+ [4].

1. The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel "for the development of multiscale models for complex chemical systems.". <https://www.nobelprize.org/prizes/chemistry/2013/press-release/>
2. Dong, D., Zhang, W., Van Duin, A. C., & Bedrov, D. (2018). The Journal of Physical Chemistry Letters, 9(4), 825-829.
3. Dong, D., Wei, X., Hooper, J. B., Pan, H., & Bedrov, D. (2018). Physical Chemistry Chemical Physics. 20, 19350-19362. Imholt, L.,
4. Dong, D., Bedrov, D., Cekic-Laskovic, I., Winter, M., & Brunklau, G. (2018). ACS Macro Letters, 7(7), 881-885.



Dengpan Dong is a fifth-year PhD student working with Prof Dmitry Bedrov on multi-scale molecular simulations, especially molecular dynamics simulations. The systems studied include alkaline fuel cells, lithium-ion batteries (electrolytes and solid-electrolyte interphase) and ion transport phenomena in ionic liquids. With five publications and three submitted papers, he has his thesis defense on October 15, 2018. Additionally, he has attended and presented on multiple academic conferences, including AIChE annual meeting, ACS annual meeting and Gordon Research Conference of Ionic Liquids.