UNIVERSITY OF CALIFORNIA
UC RIVERSIDE | Materials Science and Engineering

WINTER 2021 COLLOQUIUM SPEAKER

MARCH 3, 2021

Wednesday's 1-1:50pm ZOOM

Optimizing Li+ transport in polymer electrolytes: Insight from molecular simulations

Solid polymer electrolytes (SPEs) provide a potential to enable lithium-ion and lithium metal batteries to achieve high energy density, advanced manufacturing capabilities, and enhanced safety. However, the lack of sufficient molecular-scale insights into lithium ion transport mechanisms and reliable understanding of key correlations often limit the scope of modification and design of new materials. Moreover, the sensitivity to small variations of polymer chemical structures (e.g., selection of specific linkages or chemical groups) is often overlooked as potential design parameter. In this talk, we will use three examples to demonstrate how atomistic molecular dynamics (MD) simulations can complement experimental investigations and reveal important molecular-scale correlations between variations in polymer structures and Li+ transport capabilities. For conventional SPEs, we demonstrate that by tuning polymer chain chemical architecture a transition from strong coupling between Li+ and polymer segmental motion regime to a decoupling regime can be achieved. In single-ion conducting polymer gels, we show that small modifications of the polymer backbone significantly enhance the Li+ transport. Finally, we show how MD simulations can guide the design of novel class of SPEs comprised of supramolecular self-assembly of polyrotaxanes where the morphology of weaving linear chains and ring molecules allows for decoupling of mechanical and transport properties in SPEs.

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Dr. Bedrov received his Ph.D. in Chemical & Fuels Engineering in 1999 and has been working in the area of multiscale modeling of materials for more than 20 years in several interdisciplinary multiscale modeling centers in academia and industry. Currently Dr. Bedrov is an Associate Professor in the Materials Science & Engineering Department at the University of Utah. He is the Associate Director of the Collaborative Research Alliance with the Army Research Laboratory for Multiscale Modeling of Electronic Materials. In this Alliance, Dr. Bedrov is the Lead for the Electrochemical Devices area. He has over 160 publications in peer-reviewed journals that have over 7600 citations. His awards include the prestigious Fellowship for Experienced Researchers from German Humboldt Foundation and recognition by the University of Utah for Extraordinary Research Accomplishments.

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