

Dr. Mohammad R. Momeni obtained his Ph.D. in Theoretical and Computational Chemistry from the University of Alberta. Later, he held three postdoctoral appointments at the University of Minnesota, UC San Diego, and New Jersey Institute of Technology, where he studied the structure and dynamics of metal-organic frameworks (MOFs), guest molecules adsorptions, heterogeneous catalysis, and vibrational spectroscopy. Currently, he is an assistant professor at the University of Missouri – Kansas City, and his research interests are interdisciplinary, encompassing Theoretical Chemistry and Physics and Materials Science. He is broadly interested in developing multi-scale simulation techniques to advance the design and discovery of new materials for applications in sustainable energy conversion and storage. Over the past 15 years of active research, he has published a book chapter on the theory of photovoltaics and authored/co-authored more than 50 articles in peer-reviewed journals. Dr. Momeni is one of the leading developers of the general-purpose software package *DL_POLY Quantum* (<https://github.com/mrmomeni>).