Proceedings of the 3rd World Congress on Recent Advances in Nanotechnology (RAN'18)
Budapest, Hungary – April 10 - 12, 2018
DOI: 10.11159/icnms18.1

Molecular Simulation, Screening and Design of Nanoporous Metal-Organic Frameworks toward Potential Applications

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Metal-organic frameworks (MOFs) have emerged as a unique class of nanoporous materials and received tremendous interest over the last decade. The variation of metal oxides and the judicious choice of controllable organic linkers allow the pore size, volume and functionality of MOFs to be readily tailored in a rational manner. Consequently, MOFs provide a wealth of opportunities for molecular engineering of new nanoporous materials and have been considered as versatile candidates for many important potential applications. Nevertheless, the number of MOFs synthesized to date is extremely large, thus experimental testing alone is economically expensive and practically formidable. With rapidly growing computational resources, molecular simulation has become an indispensable tool to characterize, screen, and design MOFs. In this presentation, recent simulation studies in MOFs will be summarized toward potential applications such as methane storage, carbon capture, biofuel purification, water desalination, etc. It will be demonstrated that simulation at a molecular level can secure the quantitative interpretation of experimental observation, provide microscopic insight from bottom-up, and facilitate the development of new MOFs.

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