Invited Lecture

Accelerating the Discovery of Novel Materials for a Sustainable Society: Integrating High Throughput Screening and Machine Learning

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Porous materials especially, coordination polymers (CP) or metal-organic frameworks (MOFs) have emerged as a special class of hybrid nanoporous materials. The variation of metal oxides and the vast choice of controllable organic linkers allow the pore size, volume and functionality of MOFs to be tailored in a rational manner for designable architectures. MOFs thus provide a wealth of opportunities for engineering new functional materials and are considered as versatile candidates for storage, separation, sensing, catalysis, drug delivery and other important applications. With ever-growing computational resources and advance in mathematical techniques, molecular simulations have become an indispensable tool for materials characterization, screening and design. At a molecular level, simulations can provide microscopic insights from the bottom-up and establish structure-function relationships. This presentation will highlight on how molecular modelling combining with machine learning approach can a powerful tool in complementing experiments and thus aid in designing of new smart porous materials for storage, sensing and separation applications.[1-5]

References:

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