Improved Design of Metal Organic Frameworks for Efficient Gas Adsorption by Multi-scale Simulations

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Recently microporous crystalline metal-organic frameworks (MOFs), which are composed of metallic joints and organic struts, represent exceptional porosity (up to 90%) and high surface area (up to 10,000 m^2/g), which stimulated many studies to investigate the utility for using these materials as gas adsorbents for hydrogen (H_2), methane (CH_4), and carbon dioxide (CO_2) storage. In this talk, I will introduce how to accurately predict isotherms of the gases in the MOFs by a multi-scale simulation scheme including first principles calculations, Monte-Carlo simulation, and molecular dynamics simulation with reactive force field. And then, I will discuss several strategies for improving gas adsorption amount in the porous materials.

References

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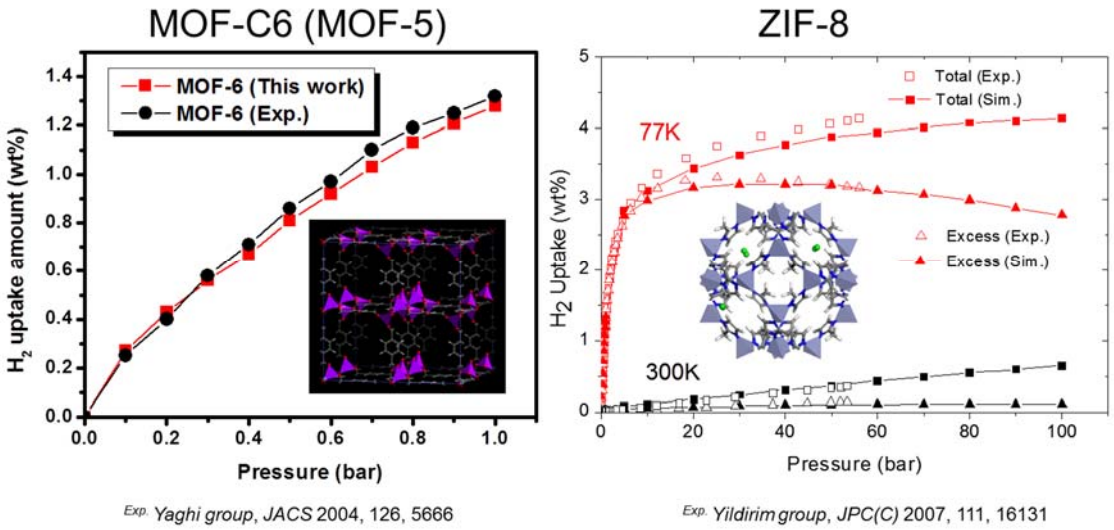
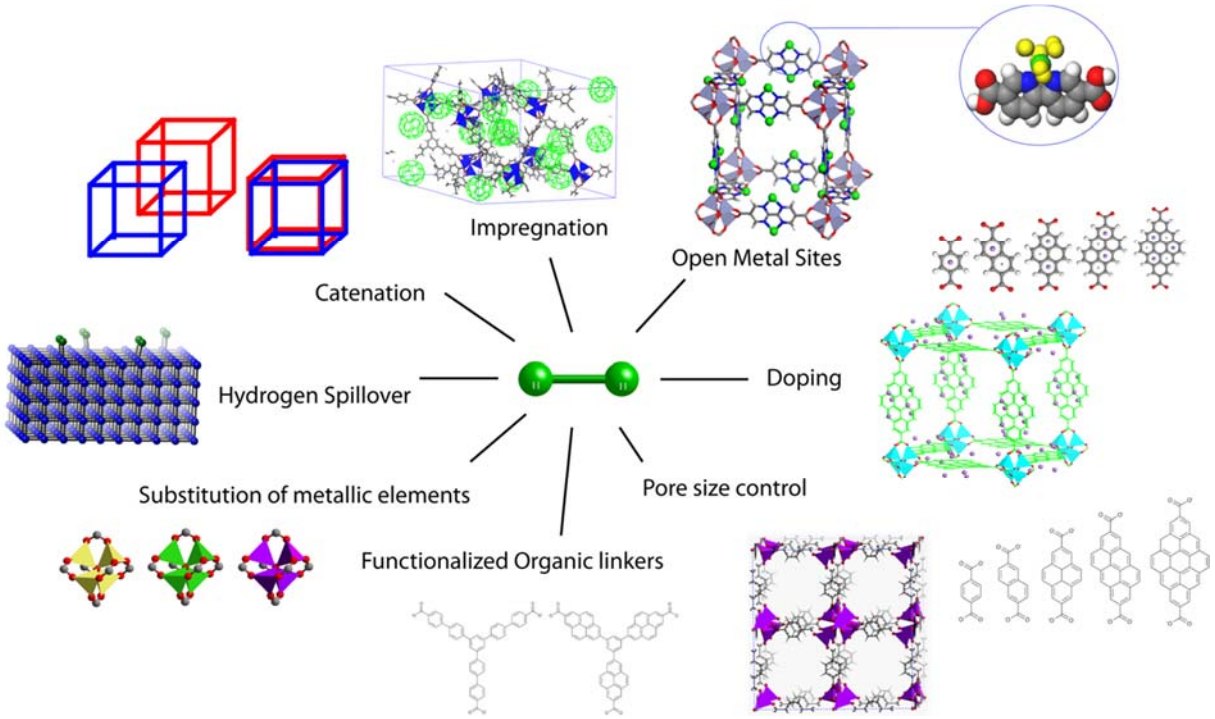


[Fig. 1] Comparison of our multiscale simulation and experiment for H_2 uptake amount in MOF-5 and ZIF-8 systems



[Fig. 2] Several strategies for improved designs of MOFs as hydrogen storage media