Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.16148

Elucidating and Manipulating Pressure-Induced Water Intrusion-Extrusion in Tunable Hydrophobic Co/Zn Bimetallic ZIFs

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The applications of porous materials are extended to the fields of vibration isolation and energy absorption. Especially, a number of porous materials have low interface affinity to fluids due to their unique nanopore structures and surface functional groups. In recent years, porous heterogeneous lyophobic systems (HLSs) are finding potential applications in energy restoring, dissipating, and absorbing. The mechanical behaviors of HLSs strongly depend on the intrusion-extrusion of the pressure-transfer medium in the micro- and mesopores. However, to the best of our knowledge, all of previously reported investigations were focused on searching promising porous materials from the documented structures via the mechanical property assessments. As a result, the mechanical performance is far away from the requirement of ideal HLSs. Besides that, thoroughly understanding the intrusion-extrusion mechanism of the liquid medium in the confined nanopores is fundamentally important to accurately predict the transport behavior and thus guide the exploration of porous materials, however, still acutely challenging. Herein, the Co-Zn bimetallic ZIFs having tunable pore sizes were employed to investigate the pressure-induced intrusion-extrusion of liquid water in hydrophobic nanoporous structures. A series of Co_xZn_{1-x}-$(MeIm)_2$ were synthesized via reaction-diffusion method and their pore sizes were successfully regulated by altering the Co to Zn molar ratio. The mechanical properties of all HLSs of {ZIF + water} were carefully evaluated and the relationship between intrusion pressure and pore size was unlocked. In combination with molecular dynamics simulations, the hydrogen bond-derived association of water molecules in the confined channel under high pressure is theoretically studied via the radial distribution function analysis and hydrogen bond calculation. The roles of pore size and hydrogen bond in synergically governing the pressure-induced intrusion-extrusion of liquid water in hydrophobic nanoporous MOFs are highlighted.