

Computational Design of Photochemically induced Water Harvesting in Metal-Organic Framework

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Harvesting water from desert air is one of the key environmental related issues in the recent years. Among various class of materials, metal-organic framework (MOF) are used the efficient material for water harvesting. In this computational study, we demonstrate that Ni-IRMOF74-III MOF structure attached with azopyridine molecules can potentially undergo photochemically induced cis/trans transition, leading to significant enhancement in the H₂O working capacity. Specifically, grand canonical Monte Carlo simulations indicate an high 0.20 kgkg⁻¹ of H₂O working capacity at 25 °C adsorption and 65 °C desorption conditions. More importantly, given that the cis/trans switching is predominantly responsible for the discrepancy in the H₂O uptake, even in the mild condition of 35 °C desorption (10 °C diurnal temperature swing), the H₂O working capacity is still very high at 0.18 kgkg⁻¹. Our theoretical findings provide a blueprint to design the next generation water harvesting materials that can operate in mild conditions to expand its applicability in different regions around the world.