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锂诱导的共价有机框架材料增强吸附热用于高效储氢

摘要

共价有机框架材料（COFs）具有高比表面积和可调节的孔结构，是极具潜力的氢气物理吸附材料。1 然而，其与氢气分子之间的相互作用过于微弱，无法充分发挥 COFs 材料的高孔隙率优势。本研究首次报道了一种通过金属掺杂增强氢气物理吸附性能的 COFs 材料。借助 TPB-DMTP-COF 材料出色的稳定性，我们在锂（Li）掺杂后成功保留了 COF 材料的孔结构，其比表面积达到 1350 m2/g。由于锂掺杂提高了材料对氢气的吸附热，材料在 77 K、80 bar 条件下的总氢气吸附量从 4.98 wt% 提升至 6.91 wt%。锂掺杂引起的增强效应不涉及化学吸附，且材料表现出优异的循环性能：在 30 bar 条件下循环 10 次后容量保持率达 99%。研究结果表明，通过后修饰调控氢气的吸附热是充分开发多孔材料潜力、实现高效氢气储存的有效策略。

关键词

共价有机框架材料；氢气存储；锂掺杂；气体吸附；吸附热

Abstract

Covalent organic frameworks (COFs) possess high surface areas and tunable pore structures and are promising candidates for H2 physisorption materials. However, their interaction with H2 molecules is too weak to take advantage of the high porosity of the COFs. Here, we report the first example of metal-doped enhanced H2- physisorption COF. By leveraging the superior stability of TPB-DMTP-COF, we can well preserve the porosity of the COF after lithium (Li) doping, yielding a surface area of 1350 m2/g. Due to the Li-doping-enhanced H2 isosteric heat, the material's total H2 uptake increased from 4.98 to 6.91 wt % at 77 K and 80 bar. The Li-doping-induced enhancement effect does not involve chemisorption, and the material shows excellent cycling performance: 10 cycles at 30 bar with a capacity retention of 99%. Our results reveal that tuning H2 adsorption heat by postmodification is a promising strategy to exploit the potential of porous materials for efficient H2 storage.

Keywords

Covalent Organic Frameworks; H2 storage; Lithium Doping; Gas adsorption; Sorption heat

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