


Alofi hydrogen energy storage

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Presently, it is unclear how material-based storage systems perform compared to compressed gas and cryogenic liquid hydrogen storage for long-duration energy storage, and what are the targets for materials to outperform them on a cost basis. Chemical H₂ storage methods convert H₂ to a storage material with high hydrogen content, such as ammonia, liquid organic hydrogen carriers such as methanol or methylcyclohexane, and metal hydrides.⁸⁻¹⁰ Ammonia and carriers are emerging as frontrunners for bulk H₂ transportation applications.^{11,12} However, they require careful thermal management to protect expensive catalysts, high temperatures to facilitate conversion, and complex purification, which may not scale or be responsive enough for power applications coupled with turbines or fuel cells.⁹

Overview of the scope of the study. (a). Proposed integration of systems analysis within material design and selection research. (b-d). Representative charge and discharge patterns for the H₂ storage system in prototypical long-duration energy storage applications.

Optimization and uncertainties of MOF performance. (a) LCOS performance profile for Ni₂(m-dobdc) at 5 \$/kg, overall porosity = 0.64 (bed and pellet porosities = 0.4), charge rate half as fast as discharge rate. Region 1 denotes the conditions with optimal LCOS for this application. (b) Breakdown of the lowest LCOS for Ni₂(m-dobdc). (c) Ranges of optimum conditions for Ni₂(m-dobdc) MOF under different assumptions of overall porosity (pellet and bed) from 0.36 to 0.84, cost of manufacturing from 2 \$/kg to 25 \$/kg (base case 0.64 overall porosity, 5 \$/kg MOF). (d) and (e) Effects of MOF manufacturing cost and overall porosity on the LCOS performance of Ni₂(m-dobdc).

However, in some cases, there may be little control over such factors, and it is therefore illustrative to identify the necessary improvement in excess H₂ uptake to be cost-competitive with a compressed gas system (SI Section S2). By applying this strategy to a scenario where the storage tank is cycled 30 times per year, we find that Ni₂(m-dobdc) can outperform 350 bar compressed gas storage in LCOS under slow charging conditions at

5 \$/kg MOF, but needs an increased uptake (>5 g/L) under fast charging scenarios (SI Figure S2).

Further, we show that for $\text{Ni}_2(\text{m-dobdc})$, the uncertainties of porosity and manufacturing cost significantly influence the optimal storage tank operating pressure (Figure 3c; input range determined in SI Section S2). For example, low porosity favors mild cooling conditions (~ 200 K) to increase uptake. For more expensive MOFs, higher pressure and lower temperatures are favored to maximize energy density and reduce sorbent usage in general. Therefore, when MOF price is around 15 \$/kg or above, the optimum conditions are found under 170 bar (highest value modeled as described in SI Section S1). These factors collectively can also have a large influence on LCOS (Figures 3d and 3e).

Another challenge related to the development of MOFs for long-duration energy storage is the magnitude of plausible materials requiring consideration due to MOF tunability. Thus, further, we show how to evaluate specific MOFs in various application settings. In the process, three types of MOFs have emerged (proposed in Table 1), described below. In the final portion of this perspective, we explore whether certain classes of MOFs are preferred candidates for specific long-duration energy storage markets under low and high electricity and land costs.

To date, most MOFs studied for H_2 storage are Type 1, including MOF-5, HKUST-1, UiO-67, ZIF-8, MIL-100, etc.^{26-30,34} They are characterized as having decent uptake under cryogenic conditions such as 77 K, and tend to favor cooled operation (SI Section S5), which is also the range that is mostly studied for these MOFs. Note that performance trends are the most generalizable for Type 1 MOFs since abundant data from multiple similar MOFs (noticeably higher uptake under cryogenic conditions) is used to develop the trend, as shown in SI Section S5.

Recently, a third type of MOF has emerged in the H_2 storage literature, which is designed to be synthesized via abundant and cheap materials (i.e., aluminum and formic acid), while retaining H_2 uptake. Type 3 MOF requires more cooling than Type 2 but reaches its peak performance under low-pressure conditions.³³ Evans et al. report a low optimum pressure range (10-40 bar), which remains high enough to transfer H_2 into fuel cells.³³ The generalization for Type 2 and Type 3 MOFs needs further evaluation, which requires more experimental data, particularly for Type 3, related to isotherm assumptions under broad temperature ranges (see SI Section S2 for discussion).

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