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Presently, it is unclear how material-based storage systemsperformcompared to compressed gas and cryogenic liquid hydrogen storage forlong-duration energy storage, and what are the targets for materialsto outperform them on a cost basis. Chemical H2 storagemethods convert H2 to a storage material with high hydrogencontent, such as ammonia, liquid organic hydrogen carriers such asmethanol or methylcyclohexane, and metal hydrides.8-10 Ammonia andcarriers are emerging as frontrunners for bulk H2 transportationapplications.11,12 However, they require carefulthermal management to protect expensive catalysts, high temperaturesto facilitate conversion, and complex purification, which may notscale or be responsive enough for power applications coupled withturbines or fuel cells.9

Overview ofthe scope of the study. (a). Proposed integration ofsystems 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 performanceprofile for Ni2(m-dobdc) at 5 $/kg, overallporosity = 0.64 (bed and pellet porosities = 0.4), charge rate halfas fast as discharge rate. Region 1 denotes the conditions with optimalLCOS for this application. (b) Breakdown of the lowest LCOS for Ni2(m-dobdc). (c) Ranges of optimum conditionsfor Ni2(m-dobdc) MOF under different assumptionsof overall porosity (pellet and bed) from 0.36 to 0.84, cost of manufacturingfrom 2 $/kg to 25 $/kg (base case 0.64 overall porosity, 5 $/kg MOF).(d) and (e) Effects of MOF manufacturing cost and overall porosityon the LCOS performance of Ni2(m-dobdc).

However, in some cases, there may be little controlover such factors,and it is therefore illustrative to identify the necessary improvementin excess H2 uptake to be cost-competitive with a compressedgas system (SI Section S2). By applyingthis strategy to a scenario where the storage tank is cycled 30 timesper year, we find that Ni2(m-dobdc) canoutperform 350 bar compressed gas storage in LCOS under slow chargingconditions at

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

Further, we show that for Ni2(m-dobdc),the uncertainties of porosity and manufacturing cost significantlyinfluence the optimal storage tank operating pressure (Figure 3c; input range determined in SI Section S2). For example, low porosity favorsmild cooling conditions (~200 K) to increase uptake. For moreexpensive MOFs, higher pressure and lower temperatures are favoredto maximize energy density and reduce sorbent usage in general. Therefore,when MOF price is around 15 $/kg or above, the optimum conditionsare found under 170 bar (highest value modeled as described in SI Section S1). These factors collectively canalso have a large influence on LCOS (Figures 3d and 3e).

Anotherchallenge related to the development of MOFs for long-durationenergy storage is the magnitude of plausible materials requiring considerationdue to MOF tunability. Thus, further, we show how to evaluate specificMOFs in various application settings. In the process, three typesof MOFs have emerged (proposed in Table 1), described below. In the final portionof this perspective, we explore whether certain classes of MOFs arepreferred candidates for specific long-duration energy storage marketsunder low and high electricity and land costs.

Todate, most MOFs studied for H2 storage are Type 1,including MOF-5, HKUST-1, UiO-67, ZIF-8, MIL-100, etc.26-30,34 They are characterized as havingdecent uptake under cryogenic conditions such as 77 K, and tend tofavor cooled operation (SI Section S5),which is also the range that is mostly studied for these MOFs. Noteperformance trends are the most generalizable for Type 1 MOFs sinceabundant data from multiple similar MOFs (noticeably higher uptakeunder cryogenic conditions) is used to develop the trend, as shownin SI Section S5.

Recently, a third type of MOF has emergedin the H2 storageliterature, which is designed to be synthesized via abundant and cheapmaterials (i.e., aluminum and formic acid), while retaining H2 uptake. Type 3 MOF requires more cooling than Type 2 butreaches 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 H2 into fuel cells.33 The generalizationfor Type 2 and Type 3 MOFs needs further evaluation, which requiresmore experimental data, particularly for Type 3, related to isothermassumptions under broad temperature ranges (see SI Section S2 for discussion).