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Cost and potential of metal-organic frameworks for hydrogen backup power supply

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25 **Abstract**

26 **Hydrogen offers a route to storing renewable electricity and lowering greenhouse gas emissions.**
27 **Metal–organic framework (MOF) adsorbents are promising candidates for hydrogen storage, but a**
28 **deep understanding of their potential for large scale, stationary backup power applications has**
29 **been lacking. Here we utilize techno-economic analysis and process modeling, which leverage**
30 **molecular simulation and experimental results, to evaluate the future opportunities of MOF-stored**
31 **hydrogen for backup power applications and set critical targets for future material development.**
32 **We show that with carefully designed charging-discharging patterns, MOFs coupled with**
33 **electrolyzers and fuel cells are economically comparable with contemporary incumbent energy**
34 **storage technologies in backup power applications. Future research should target developing MOFs**
35 **with 15 g/kg of recoverable hydrogen adsorbed (excess uptake), and could be manufactured for**
36 **under \$10/kg to make the onsite storage system a leading option for backup power applications.**

37

38 Resilient power supply has become increasingly important in today’s energy infrastructure. For example,
39 the number of power outage incidence (one hour and longer) has grown by 60% over the past five years in
40 the United States (U.S.)¹. Critical infrastructure with heavy energy consumption, such as data centers (>
41 200 TWh/yr globally) and hospitals (>210 TWh/yr in the U.S.), require uninterrupted power supply, and
42 tend to meet this requirement with diesel or natural gas generators²⁻⁵. Hydrogen-powered fuel cells can
43 offer higher energy efficiency and reliability than these fossil-fueled generators, especially when coupled
44 with on-site production of hydrogen. Hydrogen storage is necessary for this coupling, and lowering the
45 cost of stationary hydrogen storage for fuel cell applications is a significant research challenge. Given the
46 high carbon and pollutant emission profile of the current fossil-fueled generators^{6,7} and expected growth
47 in demand for backup power¹, developing reliable and sustainable backup power alternatives has become
48 increasingly critical.

49 Some concepts for low-carbon backup power employ battery banks. However, commercial-scale battery
50 backup systems are costly and are only able to sustain power for approximately 15 to 30 minutes
51 depending on the capacity^{8,9}. Advanced battery technologies (e.g., Li-ion, lead-acid, redox flow) offer
52 longer durations (2 to 10 h), but the capital cost associated with these long-duration batteries is high (from
53 1000 \$/kW for 2 hours to 3000 \$/kW for 10 hours at the 10 MW level), and falls short when compared
54 with the average 30 to 55 h power outage duration^{1,10}.

55 As noted above, hydrogen-powered fuel cell backup power systems are one emerging sustainable
56 alternative that can provide over 10 hours energy storage at high output (up to 10 MW)^{11,12}. During the
57 past decade, hundreds of fuel cell backup projects across over 40 states in the U.S. have demonstrated
58 high reliability to offer uninterrupted supply with high durability (low voltage degradation) to various
59 government and private sectors (i.e., telecommunication, railroads)^{13,14}. Combining fuel cell technologies
60 with renewably-powered electrolysis plants could offer a low-emission (carbon and other pollutants)
61 solution to backup power, avoiding up to 4–10 kg of CO and 16–18 kg of NO_x emissions per MWh of
62 backup power compared with natural gas/diesel generators¹⁵, without the need of delivering of diesel fuel
63 after each discharge.

64 But further deployment of fuel cells requires adequate hydrogen storage, which to date is energetically
65 and economically expensive¹⁶. For large-scale backup-related applications, there is a need to further
66 understanding the role of emerging hydrogen storage technologies for effectively coupling hydrogen
67 generation via electrolysis with fuel cells. This is critical as the cost and performance of the hydrogen
68 storage component have been a key factor in determining system viability when hydrogen storage in salt
69 caverns is not available^{17,18}. Furthermore, understanding and improving hydrogen's system-level energy
70 density and its economic performance, as analyzed in this study, are critical to assessing its potential for
71 larger-scale and long-duration backup solutions compared with incumbent technologies such as batteries.

72 For backup applications, physical hydrogen storage methods are theoretically the more suitable than
73 chemical storage to meet the spontaneous and intermittent needs (see details in *Scope of the Analysis*
74 Section). Metal–organic frameworks (MOFs) are a promising class of porous crystalline adsorbent
75 materials to physically store hydrogen, as they have high surface areas, large pore volumes, and in some
76 cases, strong binding sites for hydrogen¹⁹. In recent years, a significant number of studies has focused on
77 material-level optimization^{20,21} and screening^{22,23} to enhance the hydrogen storage performance of MOFs.
78 Therefore, it is critical to assess the economic potential of MOFs being used in real hydrogen storage
79 systems.

80 Techno-economic analysis (TEA) is an effective way to assess the cost performances of energy storage
81 technologies quantitatively. However, recent TEAs have mostly been focusing on chemical-based
82 hydrogen storage technologies for transportation applications^{24,25}. Limited research has been conducted on
83 sorbents, especially MOF-based hydrogen storage for large scale, stationary backup power applications.
84 Moreover, based on our previous analysis, hydrogen storage using MOFs could be more suitable for this
85 purpose than onboard transportation-based applications²⁶.

86 In this study, we combine molecular simulation, process modeling, and TEA to show that under 10 MW-
87 level applications (i.e., microgrid, distributed renewable energy generation, and community-size data
88 centers²⁷⁻²⁹), MOFs coupled with electrolyzers and fuel cells are economically comparable with
89 contemporary incumbent energy storage technologies in backup power applications. Furthermore, if
90 MOFs in the future can achieve excess uptake of 15 g/kg and could be manufactured for under \$10/kg,
91 their associated on-site storage system can be a leading option for backup power applications.

92

93 **Storage Capacity and Key Assumptions**

94 In this analysis, we set the target storage duration of 96 hours to meet the Standard for Emergency and
95 Standby Power Systems requirement for critical infrastructure established by the National Fire Protection
96 Association, which aligns with recent trends suggesting the need to be prepared for increasing power
97 outage frequency and risk in the U.S.^{30,31} In other words, the system can serve outages up to 96 hours
98 without needing to re-charge.

99 In all, this analysis centers around the energy balance on the hydrogen stored in the MOF-based backup
100 system, and the cost performance are derived from the energy and power requirements in each stage of
101 charge and discharge operation. Detailed calculations and input parameters are shown in the *Methods*
102 Section and Supplementary Notes 1 to 3. Key system-level assumptions made in this analysis are that
103 first, the temperature dependence of the heat capacity of MOFs and storage tanks is neglected
104 (Supplementary Note 1). Second, the detailed internal mass and heat transfer effects within the storage
105 tanks are recognized but not studied. Third, the system's process control is well-designed to meet the
106 steady release of hydrogen, as discussed in Supplementary Note 7. Lastly, heat exchange and insulation
107 between the ambient and the storage system are studied, but its cost effects on the broad operation
108 conditions are neglected (see supporting analysis in Supplementary Note 3).

109

110 **Performance of physical H₂ storage technologies**

111 Fig. 1 shows the system-level energy density and levelized cost of storage (LCOS) for representative
112 promising MOFs identified in previous material-level screenings^{22,32-34}. The list and selection criteria of
113 MOFs are included in the Methods section and Supplementary Note 1. Energy density is defined as the
114 amount of energy stored within a total system-level volume (the storage tanks). The levelized cost is the
115 annual-equivalent fixed capital investment and operational costs during the plant's operation life
116 normalized to the theoretical amount of energy contained in the stored hydrogen per year, excluding the

117 electrolyzers and fuel cells. The detailed calculations of these parameters are shown in Supplementary
118 Notes 1 to 3.

119 As described in the *Scope of the Analysis* Section, the conventional compressed hydrogen (Comp-H₂)
120 storage under 170 and 350 bar, and liquid hydrogen (Liq-H₂) storage under 19 K and 1 bar are used as the
121 reference cases to compare with MOF storage. Salt cavern storage, and numerous other porous geologic
122 formations presently used to store natural gas, are viable physical alternatives for storing large volumes of
123 hydrogen. However, we limit this analysis to above-ground storage solutions that can be integrated into
124 facilities without geographical limitations, thus these geological methods are not considered.

125 From Fig. 1a, Fig. 1c and Fig. 2a, we find that when the MOFs are packed loosely (under bed and pellet
126 porosities of 0.6), all of the modeled MOFs are more economical than Liq-H₂ storage, and have the
127 potential of being economically comparable with Comp-H₂ storage. Furthermore, Liq-H₂ is not suitable
128 for large-scale backup power supplies as it requires extremely low cryogenic temperature (below 20 K)³⁵.
129 As a result, significant boil-off control and handling is required, regardless of how frequently the backup
130 power system is used³⁶.

131 In terms of system-level energy density, even when packed loosely, (Fig. 1a and Fig. 1c) MOFs could
132 easily exceed compressed gas storage under the same level of pressure (170 bar) under near-ambient
133 conditions (223 K, 170 bar). When packed in a relatively dense manner at the bed and pellet porosity of
134 0.2, the system-level energy density is greatly increased due to more hydrogen being adsorbed by the
135 MOFs (Fig. 1b and Fig. 1d). Under mildly cooled and pressurized conditions (241 to 223 K, 170 bar),
136 certain MOFs, including SNU-70, V₂Cl_{2.8}(btdd) (referred to in this study as V-btdd), and Ni₂(*m*-dobdc),
137 have energy densities close to, or surpass Comp-H₂ storage under 350 bar and atmospheric temperature,
138 which demonstrates clear advantage of requiring less footprint for storage, around 30% of 170 bar Comp-
139 H₂ and 80% of 350 bar Comp-H₂ (see Supplementary Note 5). Most importantly, these MOFs exhibit high

140 theoretical potential to meet/exceed the existing DOE’s 2025 target for other smaller-scale hydrogen
141 storage applications (i.e., 1.3 kWh/L for onboard transportation³⁷).

142 While promising, note that a porosity of 0.2 is relatively low compared with pellet porosities reported in
143 bench-scale studies, and relevant studies have reported that shaping and pelletizing could influence the
144 adsorption kinetics of MOFs during bulk applications^{38,39}. Therefore, more research efforts are
145 recommended to efficiently shape and handle bulk MOF pellets while retaining their hydrogen adsorption
146 functionalities.

147 Overall, within the modeled temperature range, MOFs such as Ni₂(*m*-dobdc) and V-btdd offer the most
148 promising system-level performance as they are specifically designed to offer high hydrogen uptakes
149 under mild cooling conditions^{40,41}.

150 For all backup systems, the LCOS, as calculated in Supplementary Equation (26), is inversely related to
151 the total amount of H₂ stored per year, which can be thought of as the annual storage duration. Power
152 outages can last from minutes to multiple days. The annual duration of power outages in the U.S. under
153 regular power grid operation can reach upward of 60-70 hours.^{1,31,42} However, major events such as
154 wildfires in California, recent winter storm in Texas, and hurricanes, can extend the annual outage
155 duration to anywhere from 48 to 240 hours as a result of grid recovery.^{15,42-44} Outside of the U.S., the
156 annual outage duration is highly geographical-dependent, and can reach up to 4600 hours in extreme
157 cases for low-resilient regions.^{45,46} A backup power system may also be run to overcome “power
158 instability” issues with the grid, as well as for ancillary assistance in areas where wholesale electricity is
159 high.⁴⁷

160 Therefore, we choose 240 hours of annual storage duration as the base-case scenario for the backup-
161 focused LCOS analysis, which is primarily set to cover most outage durations in the U.S. mentioned
162 above. When the electrolyzer is powered by on-site renewables and not the grid, the system can be re-

163 charged even during a major event. Note that in extremely catastrophic cases where intermittent power
164 might not be available for over 4 consecutive days, larger storage capacities would be required beyond the
165 NFPA's 96-hour requirement³⁰. During regular times, the base case can also cover occasional critical
166 support to maintain uninterrupted and reliable power supply when there is grid stability issues⁴⁸. For the
167 MOFs considered, the minimum theoretical LCOS under the modeled storage conditions is around
168 \$4/kWh under the base-case assumptions.

169 Overall, we found that there is sparse data to guide the selection of annual hours of operation for backup-
170 focused analyses. To address this issue, we include results for various operating scenarios to demonstrate
171 the impact of different annual storage durations on system cost and performance (Fig. 1e). In particular,
172 we also include a scenario where only one full charge/discharge cycle occurs annually. The minimum
173 LCOS under this scenario is \$12/kWh for MOFs and around \$200/kWh for Liq-H₂ (See results for all
174 MOFs in Supplementary Fig. 11). Such costly systems may only be economical for critical infrastructure
175 such as a data center, which can spend a large portion of its power expenditure (up to 20%) on backup
176 supplies.⁴⁹

177 Fig. 1e shows that the LCOS can be further reduced if the system is used more frequently. During regular
178 times, annual duration of over 500-1000 hours operation start to shift the system's primary function from
179 backup power to load optimization⁴⁷, in which case future work should explore the impacts of operation
180 patterns and location on system performance.

181 Note that the details of cost performance will be affected by the actual cost to manufacture the MOFs,
182 which we discuss in later sections. For MOF-based storage, the manufacturing cost associated with the
183 MOFs at \$25/kg^{50,51} is the main cost component of the system, followed by compression and refrigeration
184 costs (Fig. 2a). This explains that from the cost perspective, higher pressure or lower temperature
185 conditions are favored within the modeled range in this study (293 K–223 K, 10 bar–170 bar). The LCOS
186 reduced primarily because less MOF is required given the increased hydrogen uptake, while the increase

187 in compression and refrigeration is not as significant. This effect is more significant under low porosity
188 conditions, where more MOFs are packed in a dense manner.

189 These relations make the 223 K and 170 bar an optimum storage condition for the modelled MOFs from
190 both the cost and energy density perspectives. In theory, lower temperature and pressure conditions can
191 be used to further enhance the energy density, but more considerations should be given on other system-
192 level complexations (see additional in Supplementary Note 9).

193 Since the capital investments of compressors and refrigerators are related to the power they are designed
194 to provide, their capital investment becomes more economical when slow charging is allowed (Fig. 2b).
195 For backup power applications, the storage system does not have to be utilized frequently. Therefore, it is
196 worth considering having longer initial charging times for the hydrogen backup storage system.

197

198 **Comparison with incumbent backup technologies**

199 As the modeled scale of operation for on-site hydrogen storage using MOFs for backup power is not
200 commercially available yet, it is important to benchmark this system with contemporary backup power
201 systems such as pumped-storage hydropower (PSH) and batteries. For this analysis, system costs for these
202 two benchmark technologies represent the capital costs normalized to the delivered power in \$/kW. The
203 operating cost is not included to circumvent the large deviation of assumptions in operating patterns.

204 Although the accuracy of the comparison requires significant in-depth modeling between the different
205 systems, Fig. 3a could imply that compared with battery technology, hydrogen storage using MOFs is
206 generally more economical when designed for longer duration storage conditions because it requires less
207 complexity to scale up. Especially at the target storage duration of 96 h for 10 MW power, hydrogen
208 backup systems involving MOFs have a high potential to outperform batteries if designed for slow
209 charging. When designed for fast charging, more expensive electrolyzers must be introduced with

210 significantly higher power (Fig. 3b), which greatly reduces the economic potential of this system. Also, it
211 is notable that hydrogen generally has a higher depth of discharge (DOD) of 90%^{34,52} or higher compared
212 to batteries (mostly around 50% to 80%)¹⁰, which can make it more competitive when compared at the
213 same storage capacity. Comparing between low carbon and emerging backup power options, the
214 economic performance of using hydrogen stored by MOFs is approximately in between batteries and
215 pumped storage hydropower for long-duration storage when allowing for slower charging (12 hours to 2
216 days). The cost range for diesel/natural gas backup generators is \$800/kW to \$1000/kW^{42,53}. Currently,
217 leading renewable energy storage methods generally require higher capital investments than diesel and
218 natural gas generators.

219 **Material development targets**

220 Fig. 4 shows the system cost for the hydrogen system packed with various hypothetical MOF materials
221 integrated with a fuel cell and electrolyzer. The rest of the MOF properties, such as the isosteric heat of
222 adsorption, heat capacity, and density, are the same as the base-case values in Supplementary Table 6.
223 The grey regions (I-II) in Fig. 4a to Fig. 4c show that when slow charging (i.e., >12 h) is allowed, MOFs
224 at the current achievable price and uptake (10 to 70 \$/kg⁵¹), isosteric heat of adsorption (-12 kJ/mol⁵⁴),
225 heat capacity (0.9 kJ/kg · K⁵⁵) and excess hydrogen uptake range (10 to 15 g/kg) have the potential of
226 outperforming batteries in terms of costs. And if the system is designed to be fully charged on the scale of
227 1 to 2 days, the required potential capital investments can be further lowered. Theoretically, this range of
228 charging time is not a concern since the backup system is not used often and is designed to supply 96 h of
229 power. However, faster charging rate will allow the system to re-charge faster when intermittent power is
230 available during the outage. Thus, future analysis on system resilience and the backup operations of
231 different scenarios will benefit setting the target charging rate.

232 For material development targets, achieving a near-future target of <\$10/kg cost (region III in Fig. 4c)
233 under the current uptake ranges (5–15 g/kg) will allow MOFs to be competitive with PSH at 48 h
234 charging. But unlike PSH (or salt cavern mentioned before), MOF-based hydrogen storage does not have
235 geological constrains, which makes it more appealing even under similar system cost.

236 Alternatively, increasing the uptake to 15–20 g/kg can help reach the same level of competitiveness even
237 if the MOF cost is slightly above \$10/kg (regions V, VI, and VIII). Excess uptake above 20 g/kg while
238 having the MOFs produced under \$10/kg will have the greatest potential. However, the benefit on
239 increasing hydrogen uptake diminishes when MOFs can be produced under low cost. Therefore, \$10/kg
240 of MOF cost and 15 g/kg of excess uptake is recommended for near-future targets under 223 K and 170
241 bar.

242 Shown in Fig. 4d to Fig. 4f, currently, MOFs' performance under closer to ambient conditions is not able
243 to compete with battery or PSH, and it is harder to achieve the same excess uptakes than 223 K and 170
244 bar. But if the same material targets are achieved, for example 5 to 15 g/kg uptake at under \$10/kg MOF
245 cost, the cost benefit is greater than 223 K and 170 bar.

246 Lowering the production cost of MOF primarily requires developing manufacturing processes with
247 cheaper raw materials^{51,56}, and can also benefit from analysis on its economy of scale given the infancy
248 stage of MOF commercialization.

249 Another critical property of developing MOFs with high storage capacity is the isosteric heat of
250 adsorption. The optimum isosteric heat under the modeled storage conditions (223 K to 298 K storage
251 temperature, 10 to 170 bar pressure) is –9.4 to –16 kJ/mol⁵⁷. Within the modeled MOFs, Ni₂(*m*-dobdc) has
252 achieved an isosteric heat of adsorption within this range, with its representative value being around –12
253 kJ/mol⁵⁴. Note that the isosteric heat of adsorption is a dynamic value that varies based on the charging
254 conditions. In this study, representative values of isosteric heats are used to calculate the cooling and

255 heating loads (i.e., integral heat of adsorption). From the cost perspective, based on the sensitivity
256 analysis in Supplementary Fig. 6 (see Supplementary Note 6), we see lowering integral isosteric heat of
257 adsorption can lead to around an additional 1 to 2 percent of cost savings by lowering the refrigeration
258 cost.

259 From the material design perspective, a greater isosteric heat of adsorption is generally accompanied by
260 the increase of hydrogen uptake. However, too strong an interaction with hydrogen eventually decreases
261 the usable hydrogen capacity due to unreleased hydrogen under the desorption pressure. Therefore,
262 beyond cost, the balance and interrelations between isosteric heat of adsorption and usable hydrogen
263 capacity, should be carefully considered for future materials development, selection and system analysis.

264 Beyond the system cost, other determining factors affect the viability of different energy storage methods,
265 such as physical footprint, safety codes and regulations, response time and durability. While our analysis
266 finds that MOF-based storage systems can meet the flow rate requirements of proton exchange membrane
267 (PEM) fuel cells in this application, for backup power applications, the metrics of measuring reliability of
268 this system should also be investigated, such as the mean time to repair and maintenance percentage.

269 **Discussion**

270 Each of these incumbent energy storage technologies discussed in this study has its own advantages and
271 disadvantages. For example, batteries could operate at a much faster start-up time (seconds to minutes),
272 and could be charged in the matter of 1 to 10 hours with recommended DOD from 50% to 80%¹⁰. PSH
273 could be charged from hours to days and has a fast switch time between charging to discharging, but has
274 geological constraints¹⁰. The successful design of a reliable, long-duration, and low-carbon backup power
275 system may in fact rely on the hybrid design of these technologies.

276 We acknowledge that broadening the market for a MOF-based systems may require faster start-up times.

277 The start-up of the MOF hydrogen backup system requires power for the unit operations, such as the

278 heater and electrical process control systems. In applications where slow start-up time of the hydrogen
279 system is a concern, small battery banks, instead of the costly ones designed for long-duration energy
280 storage (i.e., over 10 h), could be used to provide the initial momentum required to power the hydrogen
281 system in a matter of seconds. Subsequently, the hydrogen system could be self-sustained using excess
282 hydrogen.

283 Additionally, the cost performance could be greatly improved for a MOF-based hydrogen backup system
284 that is multi-functional. For example, the system could be designed for both backup power and grid
285 support,⁵⁸ allowing a 1440 annual storage duration that is flexibly distributed (e.g., approximately 60-70
286 hour backup duration per year plus up to 4-hour peak shaving per day for around 350 days per year). This
287 will reduce the LCOS to \$1/kWh for MOFs and \$17/kWh for Liq-H₂ (See complete results for all MOFs
288 in Supplementary Fig. 12). Although the LCOS in this analysis is only affected by the total storage
289 amount, the facility revenue may increase by charging when renewable energy prices are low and
290 discharging when renewable prices are high. Even under this application, we estimate that the influence of
291 MOF durability is minimal as the reported cycle lives for MOFs are in the range of 1000 to 5000.^{26,59} Such
292 applications for MOF-based hydrogen system will benefit from future studies that integrate analysis on
293 the detailed operating pattern, electricity market and renewable availability, which are highly
294 geographical-dependent⁶⁰.

295

296 **Conclusions**

297 This study translates materials properties of promising metal–organic framework (MOF) adsorbents into
298 system-level performances and costs. Our results suggest that MOFs could outperform liquid hydrogen
299 storage, and be comparable with compressed hydrogen storage (350 bar) in terms of levelized cost of
300 storage under near-ambient conditions even if the MOF-based system has a lower system-level energy
301 density. A number of state-of-the-art MOFs, such as SNU-70, V-btdd, and Ni₂(*m*-dobdc), could reach

302 system-level energy density close to compressed hydrogen storage under mildly-cooled and pressurized
303 conditions (241 to 223 K, 150 to 170 bar). Refrigeration and compression are the most expensive units
304 within the storage system besides the material cost of the MOF sorbent, and their costs could be greatly
305 reduced when slower charging is allowed. Such influence is more significant when coupled with on-site
306 generation of hydrogen from electrolyzers.

307 Compared with the contemporary renewable backup solutions (i.e., batteries and pumped storage
308 hydropower), the hydrogen backup system, including electrolyzer, MOF storage, and fuel cell, is
309 promising when supplying up to 96 hours of 10 MW backup power and allowing a recharge time of over
310 24 hours. In the near future, developing MOFs with excess hydrogen uptake greater than 15 g/kg and/or a
311 cost lower than \$10/kg could make on-site hydrogen generation and storage promising even compared
312 with pumped storage hydropower. These targets represent at least a 30% increase in near-ambient excess
313 uptake, and will require industrial demonstration of economical laboratory MOF synthesis pathways.

314 Beyond understanding the overall cost profile of this emerging technology, our study identified critical
315 areas for future research. First, developing better metrics and system-level estimation of reliability, given
316 its importance in backup power applications. Secondly, a better understanding of the effects of large-scale
317 handling and packing on the adsorption performances of MOFs is necessary, as is understanding the
318 impact of trace amounts of water from the electrolyzer system in the hydrogen on MOF durability and
319 performance. Finally, system modeling of hybrid battery-hydrogen systems and multi-functional storage
320 systems is needed to understand the potential market for MOF-based energy storage.

321 **Methods**

322 *Scope of the Analysis*

323 When considering hydrogen storage technologies for backup power application, a number of criteria can
324 be used for down selection. Importantly, the target hydrogen storage system requires rapid start-up and
325 fast release for large-scale backup power applications under unpredictable circumstances. Thus, chemical-
326 based storage, where hydrogen is chemically bonded within a carrier material, may not be the best
327 scenario because elevated dehydrogenation temperatures (i.e., 500–800 K) are required to release
328 hydrogen⁶¹, unless issues with elevated temperature are addressed with better catalyst development.
329 Furthermore, this approach could require complex system design and additional time as potential tradeoffs
330 to start and stop these systems, even if the storage of carrier material is relatively easy^{61,62}.

331 On the other hand, the major advantages of using physical hydrogen storage are its potential fast initial
332 rate and straightforward mechanism (no chemical reactions needed). Liquid hydrogen storage (Liq-H₂)
333 and compressed hydrogen (Comp-H₂) storage have been the conventional physical storage methods,
334 where hydrogen is cooled below its boiling point (20 K) or compressed to high pressure (350 bar) to
335 increase its energy density⁶³. Besides these methods, one emerging physical-based hydrogen storage
336 technology is to use adsorbents to increase the storage capacities at closer to ambient temperature and
337 moderate pressures (i.e., 100 bar) compared to Liq-H₂ and Comp-H₂ storage⁶⁴.

338 To avoid system complexity and adhere to the relevant U.S. Department of Energy (DOE)'s targets³⁷ for
339 fuel-cell backup applications (see details in the following *Backup Power System and System Boundaries*
340 *subsection* and Supplementary Note 9), this analysis focuses on modeling MOFs' storage behavior under
341 near ambient conditions (293 K to 223 K, 10 bar to 170 bar).

342 The coupled molecular simulation and process modeling approach enables TEA analysis to be conducted
343 even when experimental isotherms are not available to extrapolate the uptakes, therefore making it more

344 robust. Various promising state-of-the-art MOF materials are compared with Liq-H₂ and Comp-H₂. The
345 modeling results for the storage system are further coupled with the electrolysis and fuel cells for
346 hydrogen generation and utilization, and compared with contemporary incumbent energy storage
347 technologies such as batteries, and pumped storage hydropower (PSH), as well as the more conventional
348 diesel and natural gas generators. The results from this study can set material development targets and
349 guide future industrial applications for using MOFs to store hydrogen for large-scale backup power
350 applications.

351 *Backup Power System and System Boundaries*

352 Fig. 5a shows the scope of the study and simulation models. The on-site stationary hydrogen backup
353 system analyzed in this study consisted of three main subsystems: hydrogen generation using electrolyzer
354 stacks, hydrogen storage using MOF-packed tanks and ancillary systems, and conversion back to
355 electricity via fuel cell stacks.

356 For backup applications, it is critical to consider the different discharging options to ensure a reliable
357 power supply to the end user. Thus, in this study, we analyze several application scenarios coupled with
358 different discharging patterns, such as temperature-programmed discharge vs. natural discharge. Our
359 analysis in Supplementary Note 7 shows that MOF-stored hydrogen could easily meet the discharge
360 requirement for this application scenario. Thus, the system-level performances in this study focus mostly
361 on its storage.

362 For large-scale on-site hydrogen generation and storage applications at the scale of 10 MW, the required
363 refrigeration capacity could reach the scale of hundreds to thousands of megawatts depending on the
364 charging and discharging requirements. As this type of hydrogen application is not well understood, we
365 choose to model the system at a modest temperature range from 223 K to 293 K (−50 °C to 20 °C) for
366 several reasons. First, contemporary and classic refrigeration cost models have suggested that the cost of

367 refrigeration will increase dramatically when below 223 K⁶⁵⁻⁶⁷, which is also reflected in exemplary
368 analysis under extended temperatures (see Supplementary Note 9). Below 223 K, the refrigeration system
369 will not only increase the cost, but additional infrastructure complexations. For example, multi-stage
370 refrigeration system and multiple refrigerants need to be used⁶⁵.

371 Second, 223 K is the lowest listed backup power storage condition values by the U.S. DOE, which is set
372 based on considerations such as avoiding complexations of infrastructure, and acceptance of fuel cells in
373 varying climates³⁷. For example, rapid heating from cryogenic conditions to atmospheric condition, or the
374 warm fuel cell operation temperature is theoretically achievable, but will cause many potential concerns
375 (i.e., process control and uniformity of heating).

376 For pressure, the recommended storage pressure for large-scale above ground applications is 100 bar,
377 which is set mainly to avoid using tanks other than Type I storage tank⁶⁸. However, Type I hydrogen
378 storage tank is able to handle 170 bar storage, and recent studies have suggested 200 bar as a limit for
379 requiring more complex infrastructure (i.e., gas distribution to fuel cells)⁶⁹⁻⁷². Due to these considerations,
380 we set the base case, and the upper limit of analysis as 170 bar, since it is the pressure under which
381 several of the MOF candidates are tested while still being under the pressure limit for common Type I
382 metal-based storage tanks^{22,69-72}.

383 For the base case scenario, we assumed that the upstream hydrogen for the storage subsystem is generated
384 by an atmospheric alkaline water electrolyzer. PEM fuel cell stacks are used at the downstream to
385 generate electricity from the released hydrogen. Byproduct oxygen collection, storage, and utilization as a
386 possible source of revenue for large-scale electrolyzer systems is recognized but not modeled in this
387 study.

388 For this backup power application, the system-level targets (e.g., storage capacity, discharge duration, and
389 discharge rate) for the base case are determined assuming that the projected requirement of 10 MW of

390 power utilizes 35% of the stored hydrogen, which also accounts for fuel cell efficiency and the need to
391 store additional amount of hydrogen to supply power to the heaters during discharge (Table 1), when grid
392 energy is not available. Note that fuel cell efficiency when applied in real settings (i.e., additional loss in
393 inverters) may be lower than the 50% listed in Table 1. Thus, in reality, slightly higher storage capacity
394 might be needed. Uncertainties associated with these factors are included in the error bars of Fig. 3b and
395 are discussed in Supplementary Notes 1, 6, and 11.

396 *Operation Cycles*

397 The modeled operation cycle for this study is described in Fig. 5b to Fig. 5d. The initial state (1) of the
398 storage unit includes empty tanks under room temperature, and we assume they are under vacuum.
399 During the initial charge phase, hydrogen supplied by the electrolyzer is compressed and filled into the
400 tanks to reach state (2). During this phase, cooling of the gas and solids (tanks and adsorbents) could
401 happen simultaneously or separately (using the hydrogen gas as the coolant).
402 During the discharge phase, hydrogen is released from the tanks to the fuel cell stacks and reaches stage
403 (3), where 10% of the hydrogen is left in the tank, and the rest 90% is fed to the fuel cell at 2 bar before
404 the subsequent re-charge. During this phase, heating is provided to maintain temperature during gas
405 release from the MOF sorbents (ΔH_{des}). After each discharge, the tanks and sorbents remain at the storage
406 temperature (stage (4)), where hydrogen for the next cycle is fed from the electrolyzer, and are
407 immediately charged back to the storage state (2). After the final discharge cycle, the system naturally
408 returns to its initial state (1) for maintenance. The list of system-level targets and design specifications of
409 the base case analysis are listed in Table 2. More detailed system parameters under each operation state
410 within the charge and discharge cycle are discussed in Supplementary Note 2, Supplementary Fig. 2 and
411 Supplementary Table 2.

412 *Materials Selection and Storage Tank Models*

413 The potential materials database for this study consists of the promising MOFs from previous materials-
414 level screening studies, which have high cryogenic hydrogen uptakes, surface area, and void fraction,
415 etc.^{22,32-34}. Since the previous materials-level screenings focused on the cryogenic performance of MOFs
416 for hydrogen storage, we included additional MOFs such as V-btdd, and Ni₂(*m*-dobdc), which have
417 demonstrated promising materials-level hydrogen uptake rates under relatively high temperatures^{40,41}.
418 Experimental excess hydrogen isotherms, structures, crystal density, and pore volumes of V-btdd, and
419 Ni₂(*m*-dobdc) were used for the system and TEA modeling. For the other MOFs, the open-source
420 molecular simulation package RAPSA was used to generate the material-level hydrogen uptakes and heat
421 of adsorption at the desired storage conditions⁷³. The crystal structures other than V-btdd and Ni₂(*m*-
422 dobdc) MOFs were obtained from the Cambridge Structural Database⁷⁴.

423 The material-level hydrogen storage performances were translated into system-level bulk uptakes by
424 modeling the MOFs as packed pellets in the storage tanks under the different bed and pellet porosities.
425 The storage tank type was selected based on the target storage conditions (e.g., temperature and pressure
426 range), and corresponding design parameters and costs were modeled using the open-source Tankinator
427 tool from Pacific Northwest National Laboratory (PNNL)⁷⁵. Particularly, we selected Type I tanks
428 (aluminum tanks) for pressures under 300 bar, and Type IV tanks (all-composite tanks) for a storage
429 pressure above 300 bar. Heating and cooling in this system were achieved using Modular Adsorbent Tank
430 Insert (MATI) thin disk-shape internal heat exchangers for MOF pellets, as recommended by the
431 Hydrogen Storage Engineering Center of Excellence, and has minimum effect on the available storage
432 volume⁷⁵⁻⁷⁷. A storage and packing efficiency of 90% were used to account for the internal volume
433 occupied by the heat exchangers and other minor equipment, whose detail is discussed in “Equations (4–
434 6)” in Supplementary Note 1. The system-level storage performances, such as the specific energy and
435 energy density, were determined by combining the bulk solid-phase hydrogen uptakes for the MOFs with

436 the gas-phase storage capacities of the tanks. Details of the calculations of converting material-level
437 performance to system-level performance can be found in Supplementary Note 1.

438 *System-level Performance and Techno-economic Analysis*

439 In addition to the above-mentioned materials performances and storage tank models, we critically
440 analyzed the system-level performance of the MOF hydrogen storage system (i.e., discharge performance
441 and energy density). For the discharge performance, we studied pressure swing desorption and a robust
442 temperature-programmed depressurization scenario. Based on the system-level performances and design
443 parameters, we analyzed the levelized cost of storage (LCOS) of the hydrogen storage system
444 (Supplementary “Equation (26)”) by normalizing the capital investment and operational costs according
445 to its operating lifetime. We also utilized the system cost normalized to the output power to compare the
446 MOF hydrogen storage system with other incumbent energy storage technologies.

447 The capacity parameters related to the capital costs of the unit operations were determined based on an
448 energy balance approach between the different operating states. Instead of the conventional cost
449 performance curves in regular TEA studies and in cryogenic transportation analysis²⁶, cost models, such
450 as the refrigeration system, were adjusted to be more suitable for MW-scale applications. Note that the
451 capital costs of the compressor and refrigeration units were closely related to the target initial charging
452 and recharging requirements. Thus, for these two subsystems, we programmed the model to select the
453 higher capital investment required between the initial charging and recharging phases. Further details of
454 the economic modeling can be found in Supplementary Notes 2 and 3. All costs are installed costs, with
455 the installations included in the markup shown in the light grey bar in Fig. 2 of the main text.

456 Capital costs for all coupled electrolyzer, fuel cell, and battery systems modeled in this analysis are
457 included in Supplementary Note 11 by interpolating literature results^{10,78,79}. The cost effect caused by the

458 different types of electrolyzers and fuel cells is not modeled in detail and is counted in the uncertainty
459 range mentioned in Supplementary Note 11.

460 **Data availability**

461 The data that support the results of this study are provided in the main text and Supplementary Notes 1 to
462 11. Source data are provided with this paper.

463 **Code availability**

464 The current study uses Microsoft Excel tool (Tankinator) and open-source python software (RASPA and
465 Coolprop), whose source codes are available from <<https://www.hymarc.org/models.html>>,
466 <<https://github.com/iRASPA/RASPA2>>, and <<http://www.coolprop.org>>, respectively. All steps in the
467 analysis are described in “Equations (1) to (40)” and Supplementary Notes 1 to 11. Scripts automating the
468 analysis are available from the corresponding author on reasonable request.

469

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478

479 **Author contributions**

480 H.B., J.R.L., T.A., K.B., and M.B. conceptualized and conceived the analysis. H.B., P.P., and A.A.
481 developed the methodology. H.B. and P.P. conducted the investigation. H.F. and J.R.L. provided the
482 experimental resources. P.P. and H.F. curated the data. P.P. and H.B. wrote the original draft. H.B., P.P.,
483 A. A., K.B., H.F., M.B., J.R.L., and T.A. reviewed and edited the paper. P.P. and H.B. visualized the
484 results. J.R.L., T.A., and H.B. supervised, and obtained funding and resources for the project.

485

486 **Competing interests**

487 The authors declare the following competing interests: J.R.L. has a financial interest in Mosaic Materials,
488 Inc., a start-up company working to commercialize metal–organic frameworks for gas adsorption
489 applications. The University of California, Berkeley has been issued a patent relating to the use of Ni₂(*m*-
490 *dobdc*) on which J.R.L. is listed as a co-inventor and has applied for a patent relating to the use of V-*btdd*
491 on which J.R.L. is listed as a co-inventor. The remaining authors declare no competing interests.

492

493 **Supplementary information** is available for this paper at <https://doi.org/10.1038/xxxxx>

494 **Correspondence and requests for materials** should be addressed to H.B.

495

496 **Tables**

497 **Table 1 | Key system-level assumptions for the base case stationary on-site hydrogen storage**

498 **backup power system**

Key system-level assumptions	Value s	References
Fuel cell efficiency (%)	50	Barbir 2005 ⁸⁰ ; Barbir, 2009 ⁸¹ ; Wei et al., 2014 ⁷⁹
Additional storage for self-sustaining during discharge and other losses (%)	15	This study
Compressor efficiency (%)	70	Turton et al., 2018 ⁶⁷ ; Muthukumar et al., 2008 ⁸² ; Sdanghi et al., 2019 ⁸³
Maximum depth of discharge (%)	90	García-Holley et al., 2018 ³⁴ ; Xiao et al. 2019 ⁵² ;
Heater efficiency (%)	70	Geankoplis, 2003 ⁸⁴
Packing and storage efficiencies (%)	90	Brooks et al. 2016 ⁷⁵ ; Thornton et al. 2019 ⁷⁶ ; Tamburello et al. 2018 ⁷⁷

499

500 **Table 2 | System-level targets and design specifications for the base case stationary on-site hydrogen**
 501 **storage backup power system**

System-level targets and operation conditions	Values	References
Target storage capacity (kg H ₂)	~90,700 (varies based on storage conditions)	Projected 10 MW need with efficiencies in Table 1
Target discharge duration (h)	96	National Fire Protection Association ³⁰
Target discharge rate (kg/h)	860	This study
Annual discharge duration (h)	240	Ericson and Olis, 2019 ⁴² ; Wei et al. 2020 ¹⁵ ; EIA 2021 ³¹ ; Stone et al. 2021 ¹ ; Busby et al. 2021 ⁴³
Initial charging time (h)	12	This study
Recharging time (h)	4	This study
Feed temperature from electrolyzer (K)	353	Haug et al., 2017 ⁸⁵ ; Brauns and Terek, 2020 ⁸⁶
Feed pressure from electrolyzer (bar)	2	Haug et al., 2017 ⁸⁵ ; Brauns and Terek, 2020 ⁸⁶
Fuel cell temperature (K)	353	Wei et al. 2014 ⁷⁹ ; Wong et al., 2019 ⁸⁷
Fuel cell pressure (bar)	2	Wong et al., 2019 ⁸⁷ ; Özgür and Yakaryilmaz, 2018 ⁸⁸

502

503

504 **Figure Legends/Captions (for main text figures)**

505 **Fig. 1 | Performance of promising MOFs compared with conventional physical storage methods**

506 **a** and **b**, Fixed temperature under different pressures. **c** and **d**, Fixed pressure under different
507 temperatures. **a** and **c**, Loose packing conditions at 0.6 bed and pellet porosities ($\epsilon=0.6$). **b** and **d**, Dense
508 packing conditions at 0.2 bed and pallet porosities ($\epsilon=0.2$, 80% filled with MOF). Costs are reported as
509 installed cost. LCOS is for backup power scenario (operational parameters listed in Table 2). System-
510 level energy density for Liq-H₂ in this analysis is 2.4 kWh/L. **e**. Effect of annual storage duration on the
511 LCOS for representative MOF Ni₂(*m*-dobdc), Comp-H₂, and Liq-H₂.

512

513 **Fig. 2 | Cost breakdowns of MOFs and comparison with physical hydrogen storage methods.**

514 **a**, LCOS breakdown for MOF H₂ storage under different *T*, *P* conditions, and compressed H₂ storage
515 under 293 K and 350 bar. Pie charts show the LCOS breakdown of cases that are difficult to see based on
516 the selected *x*-axis range. “Others” represents the indirect and direct costs such as contingency,
517 engineering construction, piping, etc. Heater cost is not shown in the legend because it is negligible from
518 the plots.. “O&M” refers to operation and maintenance. **b**, The effects of initial charging and recharging
519 times on the levelized cost of storage using Ni₂(*m*-dobdc) to store hydrogen for backup power. The
520 storage conditions are 223 K and 170 bar. Note that in this study, “initial charging” denotes the first
521 charging phase. Cost for each equipment is purchase cost from the TEA model described in
522 Supplementary Notes 2 and 3, “Other” represents the indirect and direct costs such as installation,
523 contingency, engineering construction, piping, etc. Error bars include 40% markdown and 60% markup of
524 total cost accounting for variability in MOF production cost, uptake, labor, heat capacity, and heat of
525 adsorption based on sensitivity analysis (See Supplementary Note 6).

526 **Fig. 3 | System costs of MOF H₂ storage system and incumbent technologies.** **a,** The system cost of
527 MOF hydrogen storage coupled with electrolyzer and fuel cell systems for different storage capacities to
528 provide 10 MW of backup power. The costs for batteries between 20 MWh to 100 MWh are extracted
529 from ref. ¹⁰, and used to extrapolate the costs beyond 100 MWh. The costs for PSH, batteries, and
530 diesel/natural gas generators are extrapolated from ref. ^{10,42} (See details in Supplementary Note 11). **b,**
531 Breakdown of the capital system costs under different storage capacities. MOF price = \$25/kg, excess
532 uptake = 13.1 g/kg. The costs for electrolyzers and fuel cells are extracted from refs. ^{10,78,79}. Cost for
533 electrolyzer, battery, and PSH are installed cost, the installation for storage unit is included in the “other”
534 category. Error bars include 30% markdown and 50% markup of total cost accounting for variability in
535 electrolyzer, fuel cell cost, and MOF storage system (See Supplementary Notes 6 and 11).

536
537 **Fig. 4 | Current performance and material targets for H₂ backup power systems via MOF storage.**
538 Cost performance of hypothetical MOFs for the hydrogen storage system under near-ambient conditions
539 for backup power applications at different target re-charging times **a-c**, 293 K, 10 bar storage conditions:
540 **(a)** 12 h re-charge, **(b)** 24 h re-charge, **(c)** 48 h re-charge. **d-f**, 223 K, 170 bar storage conditions: **(d)** 12 h
541 re-charge, **(e)** 24 h re-charge, **(f)** 48 h re-charge. **g**, example figure showing the legends (Using 24 h re-
542 charge under 223 K, 170 bar). The lowest limit for system-level energy density is set using the
543 compressed hydrogen storage under the same temperature and pressure. The costs for batteries and
544 pumped storage hydropower (PSH) are extracted from ref ¹⁰. The costs for electrolyzers and fuel cells are
545 extracted from refs. ^{10,78,79}. Costs numbers in this figure represents installed costs for batteries, PSH, and
546 hydrogen systems.

547
548 **Fig. 5 | Process flow for the base case scenario using hydrogen stored by MOF adsorbents as**
549 **backup power system.** Dark blue color suggests how much the tanks are filled with hydrogen. **a,**

550 Overview of the main unit operations and system boundary. **b**, System boundary during the initial
551 charging and charging phases. **c**, System boundary during the discharge phase. **d**, Overview of the
552 temperature and pressure conditions for the different stages. Values in the plot are for illustration, to
553 indicate the relative pressures and temperatures in the storage tank only. See detailed values in
554 Supplementary Fig. 2 and Supplementary Table 2.

555

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