

Adsorbed xenon propellant storage: are nanoporous materials worth the weight?

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S1 Langmuir model fits

Fig. S1 displays the fits of the Langmuir model the experimentally measured xenon adsorption isotherms in the porous materials.

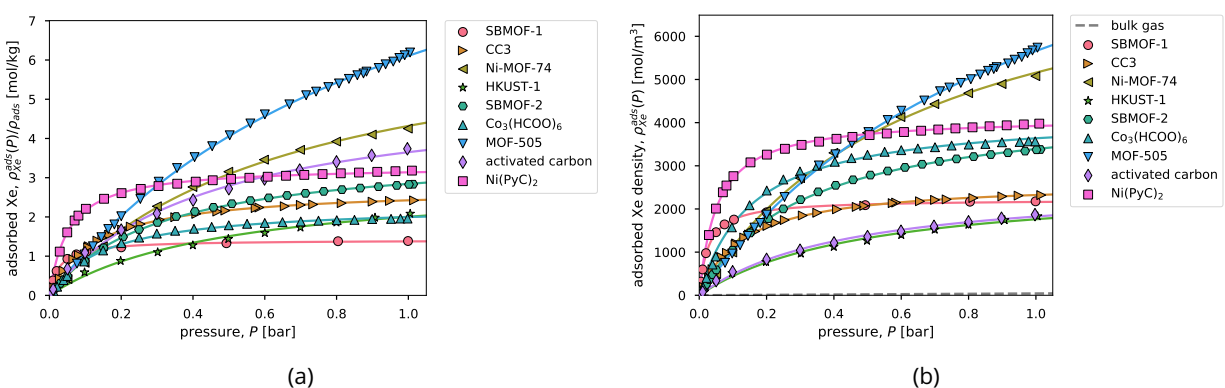


Figure S1: Experimentally measured xenon adsorption isotherms (298 K, except for MOF-505, 292 K, and Ni-MOF-74, 297 K) in the candidate materials (points) and fitted Langmuir adsorption models (curves). (a) The raw gravimetric adsorption isotherms $\rho_{Xe}^{ads}(P)/\rho_{ads}$. (b) The volumetric adsorption isotherms, $\rho_{Xe}^{ads}(P)$, obtained from the gravimetric adsorption isotherms in (a) using the density of the adsorbent, ρ_{ads} . To compare the adsorbed and bulk xenon densities, the dashed curve shows the density of the bulk gas, $\rho_{Xe}(P)$.

S2 Relationship between optimal tankage fraction and K and ρ_{ads}

Fig. S2 shows the relationship between the optimal tankage fraction in the adsorbed xenon storage system and (a) the Langmuir parameter K of the adsorbent and (b) the density of the adsorbent, ρ_{ads} .

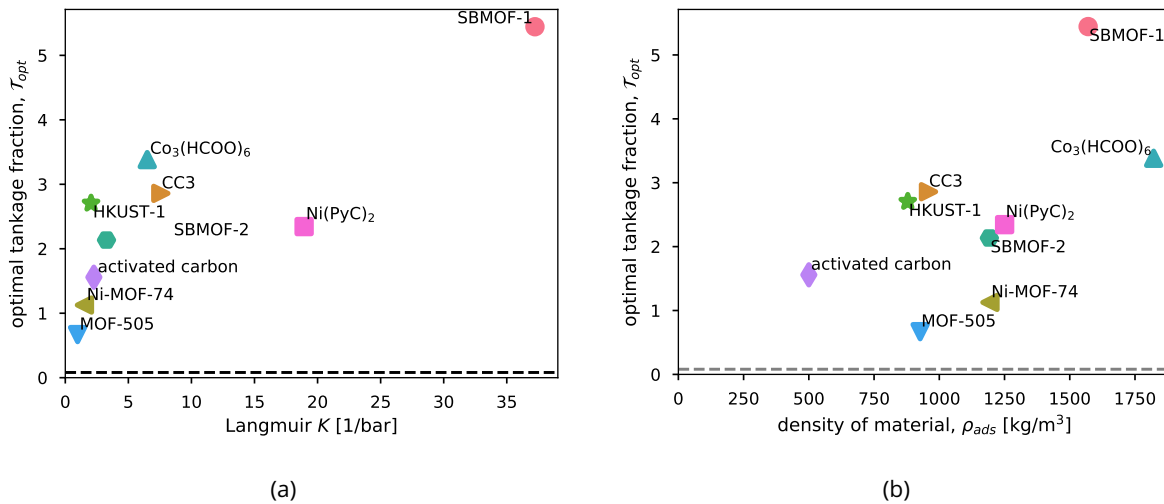


Figure S2: The relationship between the optimal tankage fraction in an adsorbed xenon storage system and the (a) Langmuir K parameter of the xenon adsorption isotherm in the adsorbent and (b) the density ρ_{ads} of the adsorbent.

S3 Relationship between adsorbed propellant storage performance

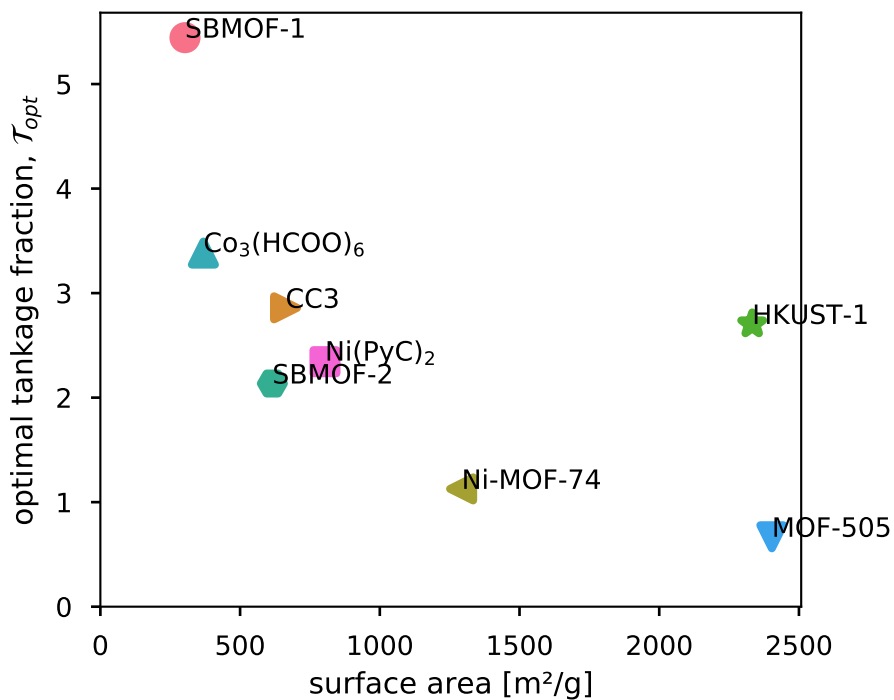


Figure S3: The relationship between the optimum tankage fraction for the adsorbed xenon storage systems and the gravimetric surface area [m^2 surface/g material] of the corresponding nanoporous materials. We computed the surface areas of the materials from the crystal structures using iRASPA [1], which defines the surface as a potential energy contour of a xenon adsorbate inside the pores of the structure defined by the Universal Force Field [2] and uses a Monte Carlo procedure to compute the area of the surface; see Ref. [1].

S4 Bulk vs. crystal density of the nanoporous materials

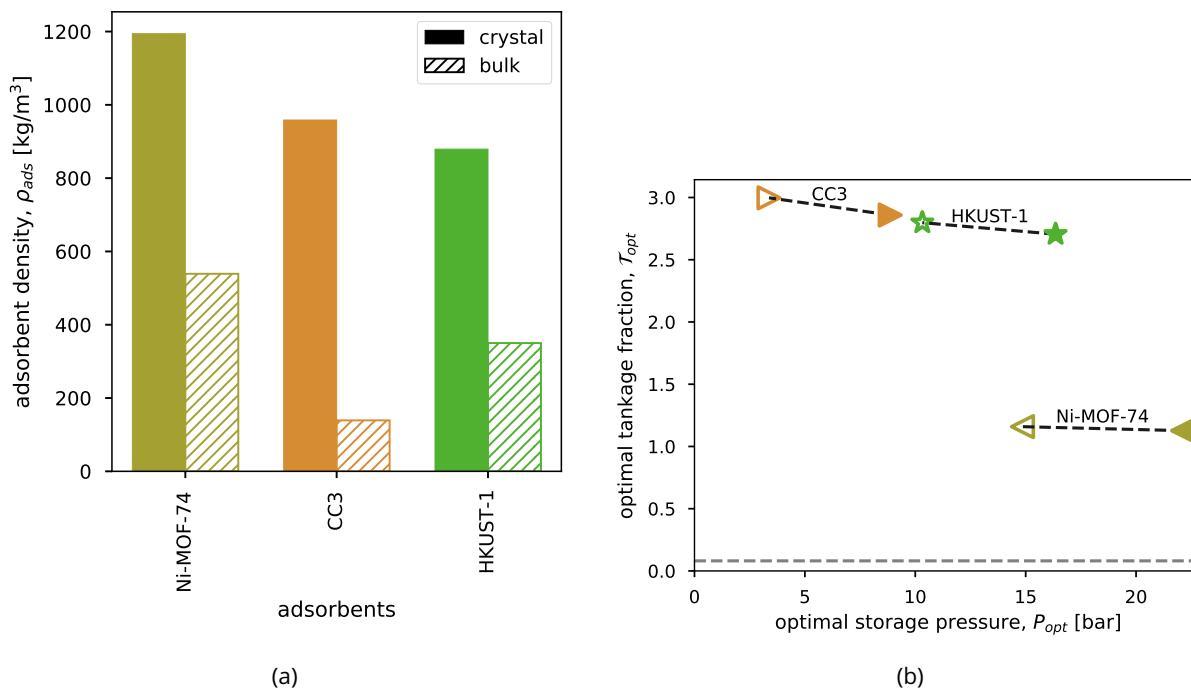


Figure S4: Investigating the impact of the approximation that the bulk density of the nanoporous material, ρ_{ads} , is equal to the crystal density. (a) A comparison of the crystal density and measured bulk/tap density [3] of CC3, HKUST-1, and Ni-MOF-74. (b) The optimal tankage fraction and storage pressure of an adsorbed xenon storage system using CC3, HKUST-1, and Ni-MOF-74, using the bulk [hollow symbols] vs. crystal density [solid symbols] as input to the model.

S5 Comparing bulk and adsorbed Xe storage systems at the same storage pressure

In the main text, we optimized the storage pressure of each adsorbed xenon storage system. However, we may wish to compare a bulk and adsorbed xenon storage system *at the same storage pressure* P . At the same storage pressure P , the difference in inverse tankage fractions in the adsorbed and bulk Xe storage systems is, using eqns. 7 and 12:

$$\left(\frac{1}{\mathcal{T}_{ads}} - \frac{1}{\mathcal{T}_{bulk}} \right) = w_{Xe} \frac{2\beta\sigma_y}{3\rho_v P} \left[\frac{1}{1 + \rho_{ads} \frac{2\beta\sigma_y}{3\rho_v P}} \rho_{Xe}^{ads}(P) - \rho_{Xe}(P) \right]. \quad (S1)$$

We write the difference in inverse tankage fractions- the mass of Xe stored per mass of storage materials (pressure vessel walls + adsorbent)- because this difference is proportional to the *net adsorption* [4] $\rho_{Xe}^{ads}(P) - \rho_{Xe}(P)$ in the adsorbent under a limiting case where the walls of the pressure vessel dominate \mathcal{T}_{ads} . i.e.,

$$\frac{1}{\mathcal{T}_{ads}} - \frac{1}{\mathcal{T}_{bulk}} \sim \rho_{Xe}^{ads}(P) - \rho_{Xe}(P) \quad (S2)$$

if:

- ρ_{ads} is very small, resulting in a light adsorbent.
- σ_y is small or $\rho_v P$ is large, resulting in a heavy pressure vessel.

Aside from this limiting case, in isolation, the net adsorption in the adsorbent is insufficient for comparing the tankage fraction of the bulk and adsorbed Xe storage systems, even when the comparison is at the same pressure (see eqn. S1).

References

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