

The rapid depletion of fossil fuels and the urgent need for sustainable energy solutions have sparked a profound scientific interest in activating small molecules. CO₂, CO, O₂, N₂, H₂ and CH₄, for example, hold immense potential as versatile resources for clean energy generation, conversion, and storage. The intricate manipulation of these molecules through ...

Here, we combined molecular structure design and electrolyte optimization (3 M ZnSO₄ with 5%NMP) in a two-pronged approach to enhance the proton storage capacity of phenazine-based organic small molecule (TAPZ) electrodes in mild aqueous electrolytes. Benefitting from the four p-conjugated amino groups provided proton conduction pathways, ...

Predicting adsorption energies of small molecules (e.g., OH, OOH, CO) on electrocatalysts involved in electrochemical reactions aids in accelerating the design and screening of electrocatalysts. ... Small-Molecule Adsorption Energy Predictions for High-Throughput Screening of Electrocatalysts J Chem Inf Model. 2023 Sep 11;63(17):5529-5538. ...

For the gas adsorption system, there could be a paradox between the adsorption of target gas and water vapor. So, the adsorption behaviors of different working pairs; energy conservation and energy storage in the zeolite adsorption stage; and the heat and mass transfer properties of different zeolites and adsorbates have to be studied in-depth.

Structures of H₂-adsorbed clusters that are in the adsorption energy range of -6 to -18 kJ mol⁻¹ in the order of CuAg₄, Cu₆, Cu₅Ag, Cu₄Ag₂, Cu₃Ag₃, Cu₂Ag₄, CuAg₆, Cu₅ ...

Chapter One - Solid-state NMR of small molecule adsorption in metal-organic frameworks (MOFs) Author links open overlay ... gas storage, catalysis, and others can be envisioned. ... (20) $D(T) = D_0 e^{-E_A/RT}$, where D_0 is the diffusivity at infinite temperature, E_A the activation energy and R the ideal gas constant. This description is ...

With growing demands of energy and enormous consumption of fossil fuels, the world is in dire need of a clean and renewable source of energy. Hydrogen (H₂) is the best alternative, owing to its high calorific value (144 MJ/kg) and exceptional mass-energy density. Being an energy carrier rather than an energy source, it has an edge over other alternate ...

Here, by using neutron powder diffraction, volumetric gas adsorption, inelastic neutron scattering and first-principles calculations, we investigate a magnesium borohydride ...

Developing a safe, affordable and efficient way of storing H₂ is a key priority in hydrogen energy research. Current fuel cell vehicles, such as the Toyota Mirai, use 700 bar compressed H₂, which provides a gravimetric H₂ capacity of approximately 5.7 wt% and a volumetric capacity of 40 g H₂ l⁻¹ [1]. Compressed H₂ storage offers quick refill times and ...

Metal-organic frameworks (MOFs) are a class of three-dimensional porous nanomaterials formed by the connection of metal centers with organic ligands [1]. Due to their high specific surface area and tunable pore structures, and the ability to manipulate the chemical and physical properties of such porous materials widely through the substitution of metal nodes ...

1 INTRODUCTION. There is a current need for economically viable and higher performing energy storage solutions. As societies move away from fossil fuels, increasing attention is paid to converting renewable energy sources to electrical energy that can be stored in an efficient energy storage system. 1-3 Owing to their high-energy density and high-power, lithium-ion batteries ...

zone is sampled with a 6 × 6 × 1 k-mesh grid and a kinetic energy cutoff of 450 eV is adopted. The adsorption energy E_a of a molecule on antimonene is calculated as $E_a = E_{Sb+mol} - E_{Sb} - E_{mol}$, where E_{Sb+mol} , E_{Sb} , and E_{mol} are the energies of the molecule-adsorbed antimonene, the isolated antimonene, and the molecule, respectively.

NMR study of small molecule adsorption in MOF-74-Mg M. G. Lopez, 1 Pieremanuele Canepa, 1 and T. Thonhauser 1, a) Department of Physics, Wake Forest University, Winston-Salem, NC 27109,

Molecular Simulations of Adsorption and Energy Storage of R1234yf, R1234ze(z), R134a, R32, and their Mixtures in M-MOF-74 (M = Mg, Ni) Nanoparticles ... which was because that the small molecule structures of R32 and R134a could effectively utilize the pore structure in MOF-74 to increase the adsorption quantity. With the increase in ...

Thermochemical energy storage holds great promise in solar energy applications, and MgCl₂ hydrate salt is considered a promising material for medium and low-temperature thermochemical energy storage. Understanding the adsorption behavior of water molecules in MgCl₂ hydrate salts and uncovering the underlying mechanisms are crucial for ...

A large enough value for adsorption energy shows potential storage or catalytic application for the adsorbed gas. Download: Download high-res image (353KB) ... for a small gas molecule. Equation (4) shows that a low value of adsorption energy of each gas on the material surface leads to a long recovery time, resulting in poor sensing material ...

As a result, the advances in producing extremely small nanopores shall boost hydrogen storage capacity in nanopores significantly. Download: Download high-res ... The adsorption density while energy parameter is

200 K is over 20,000 ... pressure, and molecule-wall interaction. Adsorption density could be 10 times that of bulk hydrogen density ...

Coal bed methane (CBM) is mainly composed of CH₄ and a small amount of CO, CO₂ and N₂. A large number of experts and scholars have carried out a large number of experimental and simulation ...

Table 1. Adsorption energy (E_{ad} in meV), electron transfer from the InSe monolayer to the adsorbed molecule (Q in e), the nearest distance between the adsorbed molecule and the InSe monolayer (d_{X-Se} in Å). The doping style of the molecule for the InSe monolayer is listed in the last column. For the electron transfer, the positive value means that ...

Hydrogen energy has garnered significant attention in recent years as a solution to address the global energy crisis and environmental pollution. While water electrolysis stands out as the most promising method to produce green hydrogen, the sluggish reaction kinetics of the oxygen evolution reaction (OER) on the anode increases the cost of hydrogen production. ...

In the following, examples of small molecule adsorption will be described organized via different adsorbed molecules. The different options for characterization provided above will be addressed. ... Hydrogen adsorption is of current interest, for instance, for energy storage applications. In terms of NMR spectroscopy, H₂, D₂ or HD can be ...

Hydrogen energy has garnered significant attention in recent years as a solution to address the global energy crisis and environmental pollution. While water electrolysis stands out as the most promising method to ...

The structure and morphology of the utilized PTCDI were firstly characterized (Figs. S1 and S2). X-ray diffraction (XRD) patterns clearly show typical characteristic peaks of PTCDI crystal structure, which can be assigned to (011), (021), (002), (11 2 (-)), (12 2 (-)), and (140) planes. Scanning electron microscope (SEM) image of the PTCDI in the inset of Fig. S1a ...

Porous adsorbents, including activated carbons, zeolites, silicas, and newer materials such as metal-organic frameworks, have been investigated extensively for gas storage and separation applications. A key consideration is the performance of a material in terms of both its pure gas and multicomponent adsorption behavior, and so measuring accurate gas ...

storage (ECS) devices, such as small molecule (water, carbon dioxide and nitrogen) electrolyzers, rechargeable metal-air ... 2.2 oxygen adsorption energy (Fig. Scaling Relations The electrocatalytic activity is to a large extent determined by the binding strength between the reaction intermediates

The adsorption of small-molecule gases (NO₂, SO₂, NO, H₂, N₂, O₂, CO, CO₂, H₂O, H₂S, and NH₃) on GeS was studied using first-principles density functional theory (DFT). The study revealed that, among the

small-molecule gases, NO₂, SO₂, and NO present the highest adsorption energies of 0.746 eV, 0.466 eV, and 0.412 eV, respectively. Moreover, ...

The effect of the BNNT surface curvatures on gas adsorption was investigated and found that strong curvatures can significantly change the adsorption potential energy surfaces [38]. Adsorption of H₂ molecules on armchair (3,3) and zigzag (5,0) BNNTs and their Mg doping derivatives was observed and H₂ storage capacities up to 9.65 % and 8.77 % were found [39].

The depth of the physisorption well for the hydrogen molecule is actually very small (in some cases negligible), but this is not the case for other molecules and does not alter the basic conclusions regarding dissociative adsorption that result from this model; namely that the process may be either activated or non-activated depending on the exact location of the curve ...

MIL-88A metal-organic framework with the unsaturated Fe metal coordination sites has demonstrated to be a promising material for gas storage and capture. However, the hydrogen storage capacity of MIL-88A has to be improved to meet the practical level at the ambient conditions. In this research, we elucidated the effects of transition metal substitution ...

A predictive model for quantitative determination of the adsorption energies of small molecules on metallic materials and oxides is proposed, by using a linear combination of ...

Because of the higher adsorption energy, cyclen will be more easily adsorbed on the surface of Zn than H₂O. Moreover, the adsorption energy of cyclen on Zn (002) is the highest, inducing the preferential and uniform deposition of Zn²⁺ along the Zn (002) face. The electric double layer (EDL) capacitance of the Zn anode in two types of ...

adsorption on small gold-copper binary clusters was also reported in 2015 by Zhao et al.³¹ Very recently, Galvez-González et al. reported H₂ adsorption on Au- and Pt-doped copper clusters with the size of four atoms.³² The research focusing on the potential use of mixed transition-metal nanostructured materials for hydrogen storage is ...

Exceptionally large surface area and well-defined nanostructure are both critical in the field of nanoporous carbons for challenging energy and environmental issues. The pursuit of ultrahigh ...

Hydrogen molecule can be dissociated into atoms on waved graphene under high compression by overcoming a weak chemical adsorption energy as small as of 0.06 eV. The positive chemical adsorption energy of oxygen molecule on waved graphene is greatly reduced, leading to exothermic reaction with a binding energy of -0.68 eV.

(d) Binding energy of Zn²⁺ with different compounds (H₂O, TMP, SO₄²⁻) calculated by DFT. (e) The

electrostatic potential maps of the H_2O and TMP molecules. (f) The scheme of EDL structure before and after the introduction of TP. (g) The adsorption model of TMP and H_2O molecules on different crystal planes of Zn. (h) the Zn-O bond ...

identify the fundamental determinants of adsorption energy but also pave the ways of fast estimate of adsorption energy. Intuitively, the adsorption energy should be a function of the

Molecular separation is an essential component in many human daily activities and multiple industrial, medical, and environmental processes, such as water purification, oil and gas refining ...

Dissociation, the breaking of an adsorbate molecule into different atoms or molecules, is problematic because the resulting adsorption energy is no longer consistent with what is of interest, i.e ...

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