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Multiscale simulation approach to heat and mass transfer properties of nanostructured materials for sorption heat storage

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Abstract

Thermal storage devices are becoming crucial for the exploitation of solar energy. From the point of view of seasonal energy storage, the most promising technology is represented by adsorption thermal batteries, which allow storing energy without heat loss with time. The improvement of thermal batteries design is related to a better understating of transport phenomena occurring in the adsorption/desorption phases. In this work, we discuss an efficient computational protocol to characterize adsorbent materials, in terms of both heat and mass transfer proprieties. To this purpose, a hybrid Molecular Dynamics and Monte Carlo method is developed. The proposed model is then tested on two types of 13X zeolite, with 76 and 88 Na cations. The results obtained, such as adsorbate diffusivity, adsorption curves, and heat of adsorption are validated with the literature. Finally, in the view of a multiscale analysis of sorption thermal storage devices, the possible use of the simulation outputs as inputs of thermal fluid dynamics models of adsorbent beds is discussed.

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Keywords: Thermal Storage; Nanoscale Heat Transfer; Sorption Heat Storage; Zeolite; Water; Multiscale Simulations

1. Introduction

The usage of renewable energy sources (especially solar energy) is exponentially growing in the last years, due to both economic and environmental reasons [1]. One of the major bottlenecks that is currently limiting a more extensive

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diffusion of solar technologies is the mismatch between energy availability and user demand, due to the intrinsically intermittent and unpredictable nature of solar source [2, 3]. Energy storage systems are appropriate ways to provide equilibrium between energy supply and demand, with the aim to make accessible everywhere and every time the electrical and thermal energies produced when and where renewable sources are available, at least at a regional scale. In particular, the development of economically feasible, efficient and reliable thermal storage systems is crucial for the sustainable and efficient use of solar energy source [4, 5]. Sorption heat storage has the potential of loss-free, more compact and efficient thermal storage systems respect to traditional sensible and latent heat storage [6, 7]. However, the multiscale nature of nanostructured materials involved in sorption processes (e.g. zeolites, metal-organic frameworks, silico-aluminophosphates) is limiting their commercial exploitation, due to difficulties in predicting macroscopic material properties strongly affected by nanoscale mechanisms [8-15].

In fact, sorption heat storage systems are simulated by models spanning from macroscopic to sub-nanometer scales. System simulations are used to estimate the overall energy performances of heat storage systems coupled with solar source [16-18]. These system-level models are typically based on 1D approximations, where the properties of materials for sorption heat storage are taken from either theoretical considerations or experimental correlations [19, 20]. Continuum simulations are then employed to model and optimize the adsorption kinetics in sorption reactors [21, 22]. Instead, nanoscale properties of sorbent materials can be investigated by atomistic simulations, such as molecular dynamics or Monte Carlo [23-25]; whereas, quantum approaches are employed to generate force-field parameters for atomistic simulations and to study fundamental interactions at the sorbent-sorbate interface [26, 27].

In this work, we systematize a multiscale simulation approach to investigate materials for sorption heat storage. Thanks to both Monte Carlo (MC) and Molecular Dynamics (MD) simulations, this method allows computing adsorbate diffusivity, adsorption curves, and heat of adsorption of nanoporous materials for thermal storage. As a test case, the properties of water adsorbed on 13X zeolites with a different amount of Na cations are studied and validated with the literature.

2. Methods

A hybrid MD/MC protocol is adopted to study heat and mass transfer properties of nanoporous materials for sorption heat storage.

As a test case, water sorption on 13X zeolite with different Na cation concentrations is considered: the strong hydrophilic behavior of its nanopores makes it an excellent material for sorption heat storage devices [28]. In particular, 13X zeolite with either 76 (Fig. 1a) or 88 Na cations per unit cell is considered in these simulations. Note that the water sorption on zeolite pores is strongly affected by concentration and position of Na cations within the framework [29, 30], which should be placed in the crystal structure according to the Lowenstein's rule [11]. The unit cell of zeolite is duplicated along *x,y,z* axes to obtain a cubic simulation domain with 5.02 nm edge (2x2x2 unit cells). The force-field adopted in the atomistic simulations is made of nonbonded (*i.e.* van der Waals and Coulomb interactions) and bonded (*i.e.* covalent bonds) potentials, with Na cations free to diffuse within the zeolite framework. Bonded interactions are modelled by harmonic terms in the MD simulations [11]; whereas, nonbonded interactions are mimicked by 12-6 Lennard-Jones and Coulomb potentials, respectively [31]. The considered water model is TIP4P (Fig. 1b) [31].

After energy minimization, the adsorbent-adsorbate couple is simulated by Gran Canonical Monte Carlo simulations to compute equilibrium properties such as adsorption curves (periodic boundary conditions; 2 million steps; temperatures from 300 to 350 K; pressures from 10^{-4} to 3.5 kPa). MD simulations are performed to compute the heat of adsorption and the self-diffusivity of water within the zeolite structure (multiple hydration levels by random particle insertion; 1 ns NVT equilibration followed by 2 ns NVT production run). Finally, heat of adsorption is computed from the average adsorbent-adsorbate (nonbonded) interaction energies during the simulated trajectory; whereas, isotropic self-diffusion coefficient of water nanoconfined in the zeolite pores is estimated by mean square displacement and Einstein’s relation [32-36]. Further details on the simulation methods are reported elsewhere [11].

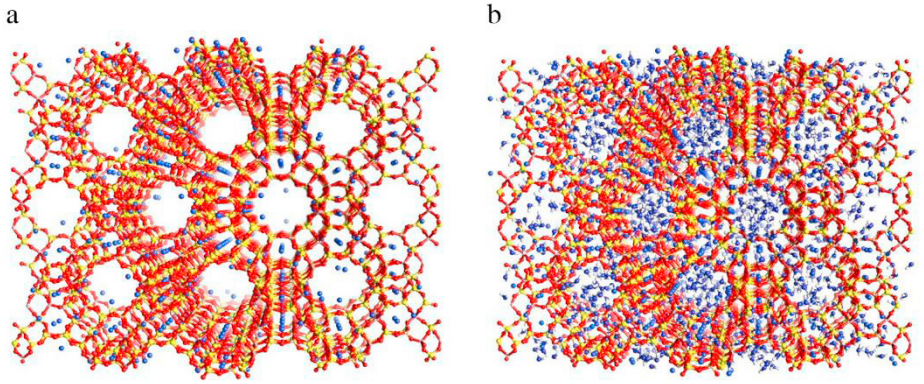

Fig. 1. (a) Dry and (b) hydrated 13X zeolite with 76 Na cations considered in the simulations.

3. Results

3.1. Adsorption curves

Adsorption curves represent the mass of adsorbed water molecules per fixed amount of zeolite (kg_W/kg_Z), at different partial pressures (p or p/p_0, being p_0 the saturation pressure).

First, adsorption isotherms are crucial to draw the thermodynamic cycle of a sorption heat storage device in the Clapeyron diagram [11]. Here, adsorption isotherms (300 K) of 13X zeolites with 76 or 88 Na are computed by MC simulations. Results in Fig. 2a highlight that simulations (dots) are well-fitted (R^2>0.95) by Toth equation (lines), which is a semi-empirical expression to model type-I adsorption isotherms [37]. Furthermore, the higher hydrophilicity of zeolite framework due to larger Na concentration leads to an isotherm shifted towards lower adsorption pressures. As reported in Fig. 2b, these simulation results are in good agreement with experiments available in the literature (300 K, 13X zeolite with 76 Na) [31].

Second, adsorption isobars allow evaluating the typical regeneration process of zeolite-based thermal batteries. In fact, either temperature increase or partial pressure decrease induce adsorbed water molecules to evacuate from the zeolite nanopores and, thus, to recover the thermal energy potential of the material. Such a behavior is observed in Fig. 3, where adsorption isobars are computed for 13X zeolite with 76 Na.

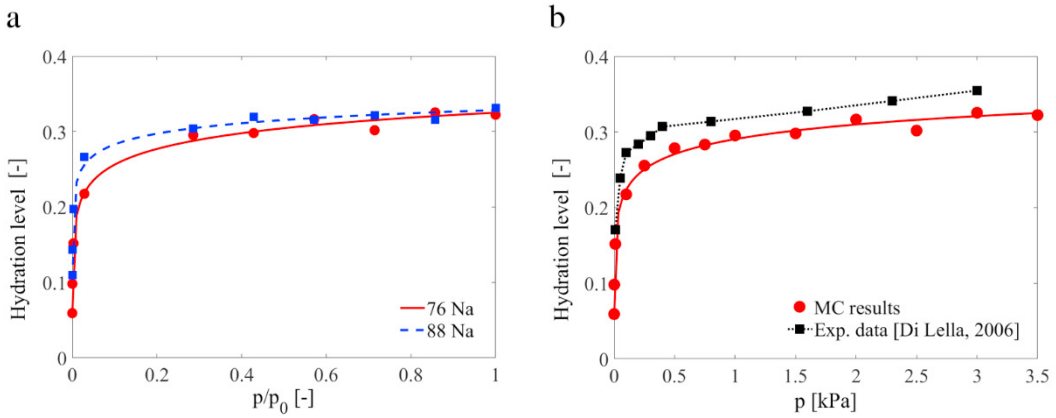

Fig. 2. (a) Adsorption isotherms (300 K) of 13X zeolites with different Na concentrations: simulation results (dots) are fitted by Toth equation (lines). (b) Comparison between simulation results and experimental evidences by Di Lella and colleagues (13X zeolite with 76 Na) [31].

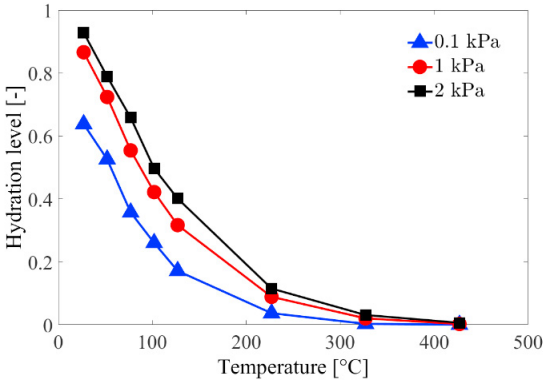

Fig. 3. Adsorption isobars for 13X zeolite (76 Na), as obtained by MC simulations.

3.2. Heat of adsorption

Molecular dynamics simulations are then performed to compute the isosteric heat of adsorption (q) of the water-13X zeolite adsorbent-adsorbate couple, which corresponds to the enthalpy released during the adsorption process (Δh). By considering negligible kinetic energy contribution (*i.e.* low operating temperature), the isosteric heat of adsorption has been estimated as $q=\Delta h \approx U_{WZ}-U_{WW}$ [38], being U_{WZ} and U_{WW} the average water-water and water-zeolite interaction energies measured in the MD trajectories, at different hydration levels (Fig. 4a). Results in Fig. 4b for 13X zeolite with 76 Na show that, in good agreement with experimental and simulation evidences [31], heat of adsorption tends to decrease with nanopores hydration. In fact, the first molecules entering the zeolite nanopores can adsorb to sites with larger water–zeolite potential wells, hence releasing a larger amount of kinetic energy. Successive molecules progressively adsorb on sites with reduced potential wells, therefore generating smaller enthalpy releases.

Furthermore, the influence of temperature on q is investigated in the range 300–700 K. As shown in Fig. 4c, the released enthalpy decreases with temperature: in fact, due to their larger kinetic energy, water molecules can adsorb on a progressively reduced number of adsorbent sites [39]. Moreover, heat of adsorption is enhanced by stronger water-zeolite interactions, as demonstrated by 13X zeolites with more Na cations and thus hydrophilicity (Fig. 4d).

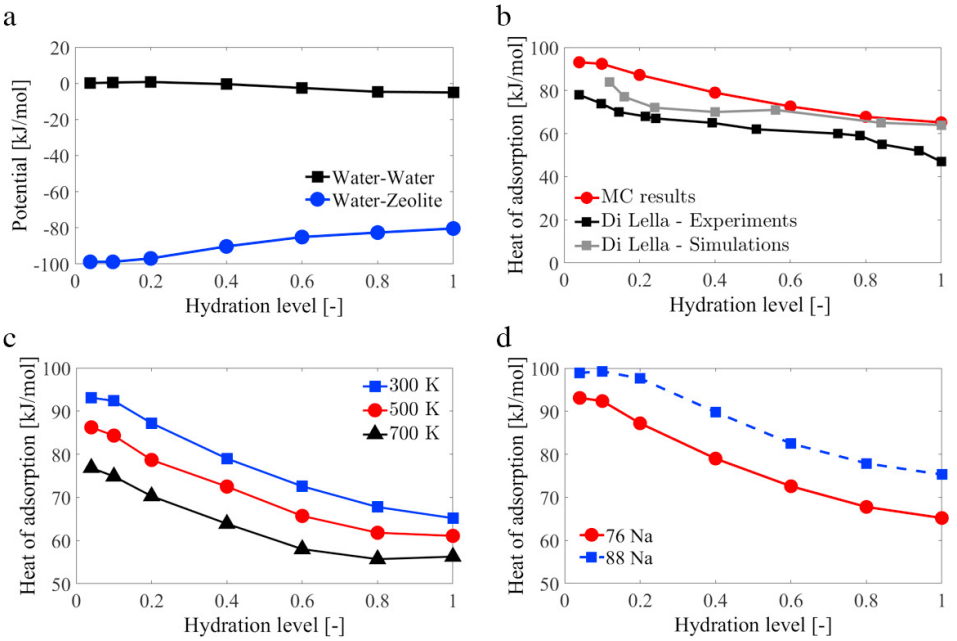

Fig. 4. (a) Average interaction potential between water-water and water-zeolite molecules (13X zeolite with 76 Na, 300 K). (b) Heat of adsorption of water on 13X zeolite (76 Na, 300 K): MD results are compared with experimental and simulation measures by Di Lella et *al.* [31]. (c) Heat of adsorption of water on 13X zeolite (76 Na) at different temperatures. (d) Heat of adsorption of water on 13X zeolites at 300 K.

3.3. Water diffusivity

Mass transport of adsorbate through the adsorbent material can be investigated by computing the self-diffusion coefficient (diffusivity) of water molecules adsorbed on the zeolite pores. Self-diffusion coefficient is a measure of mobility of water molecules, and it can be estimated – by Einstein's equation – from the mean square displacement of water molecules during MD trajectories [40].

First, in Fig. 5a, the water diffusivity at different pore hydration levels is reported for 13X zeolites with 76 and 88 Na, respectively. Results show that water diffusivity increases with hydration at low pore fillings (from 0 to 0.6); whereas, an inverse behavior is observed at higher ones (from 0.6 to 1.0). On the one side, the initial increase may be due to larger energy of adsorption – and thus mobility reduction – of water molecules at low hydration levels (see Fig. 4a), which progressively decays with increasing pore fillings. On the other side, larger pore fillings lead to enhanced water-water interactions and thus collisions, which have a detrimental effect on diffusivity. Furthermore, Fig. 5a highlights also the characteristic mobility reduction of water molecules with more hydrophilic (*i.e.* 88 Na) nanoconfining surfaces [9]. Note that these results are in qualitative agreement with water diffusivities obtained from Quasi Elastic Neutron Scattering experiments [41].

Second, water diffusivity increases with temperature because of the higher kinetic energy of adsorbate molecules (see Fig. 5b, 13X zeolite with 76 Na). Such a relation can be interpreted by Arrhenius equation [42], that is

$$D(T_i) = D(T_0) \cdot exp\left(-\frac{E_a}{RT_i}\right), \tag{1}$$

where: $D(T_i)$ and $D(T_0)$ are the water diffusivities at the considered and reference (e.g. 300 K) temperature, respectively; E_a is the activation energy of the material confining the motion of water molecules; R is the gas constant. By fitting MD results to Eq. 1 (for example, see Fig. 5c for 0.1 and 1.0 pore hydrations), a decreasing activation energy of water self-diffusivity in 13X zeolite (76 Na) is observed, namely a sharper relation between water self-diffusivity and temperature at low pores fillings.

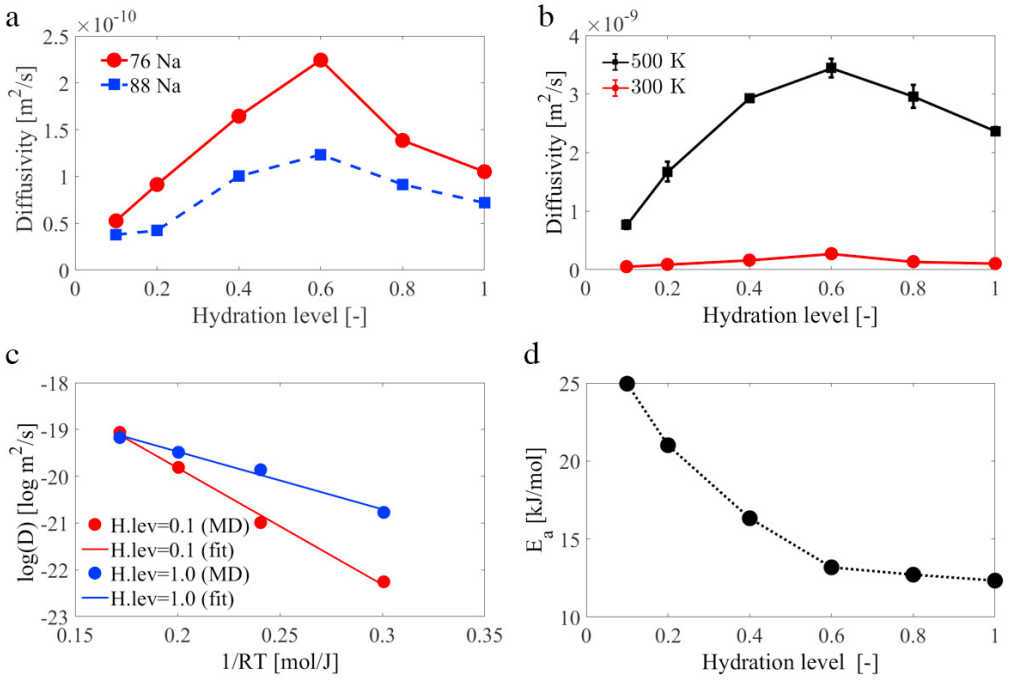

Fig. 5. (a) Self-diffusion coefficient of water adsorbed on 13X zeolites (76 Na; 88 Na), at 300 K and different hydration levels. (b) Self-diffusion coefficient of water adsorbed on 13X zeolite (76 Na), at different temperatures and hydration levels. (c) Fitting and (d) activation energy of self-diffusivity of water in 13X zeolite (76 Na), according to Arrhenius equation (Eq. 1).

4. Conclusions

A hybrid MC/MD method for characterizing heat and mass transfer properties of adsorbate-adsorbent materials for sorption heat storage has been tested in the case of water-13X zeolite couple. The adsorbate diffusivity, adsorption curves, and heat of adsorption obtained by simulations have shown good agreement with the experimental and simulation results in the literature.

To assess the capability of the simulation method to quickly explore different configurations, the effect of crystal modifications on the physical proprieties of the adsorbent material has been investigated by comparing simulation results of 13X zeolites with 76 or 88 Na cations, respectively. Results show that an increasing number of cations involves larger nonbonded interactions between adsorbed water and zeolite, which in turn lead to higher heat of adsorption and reduced water mobility (diffusivity). Such atomistic simulations allow estimating several engineering properties of novel adsorbate-adsorbent with promising performances for heat storage applications. For example, the (thermal) energy that can be ideally stored per unit volume of adsorbent material (e, kWh/m^3) can be estimated as

$$e = \frac{q \cdot \rho_{bed} \cdot \omega}{18 \cdot 3.6}, \tag{2}$$

where: q is the heat of adsorption for a certain hydration level (kJ/mol); ρ_{bed} is the density of adsorbent bed, which depends on the size of adsorbent particles and the packing level (e.g. 650 kg/m^3 [43]); ω is the considered hydration level (kg$_W$/kg$_Z$). By considering the MD results at full pores hydration (see Fig. 4d), Eq. 2 estimates an energy density approximately equal to 220 and 250 kWh/m^3 for the 13X zeolite with 76 and 88 Na cations, respectively. These results are close to experimental values reported in the literature [43].

Considering a multiscale overview (see the scheme in Fig. 6), the heat storage potential of novel adsorbent materials can be explored by first computing heat and mass transfer properties at the fundamental level (MD/MC simulations). Then, these nanoscale quantities can be used as inputs of classic thermal fluid dynamics (continuum) models of adsorbent beds (e.g. [44, 45]), in order to estimate the engineering performances of the whole thermal battery. The perspective is, therefore, a quick (and thus massive) computational assessment of promising materials for sorption heat storage, in order to improve the time-to-market (and thus commercial widespread) of novel adsorbent materials.

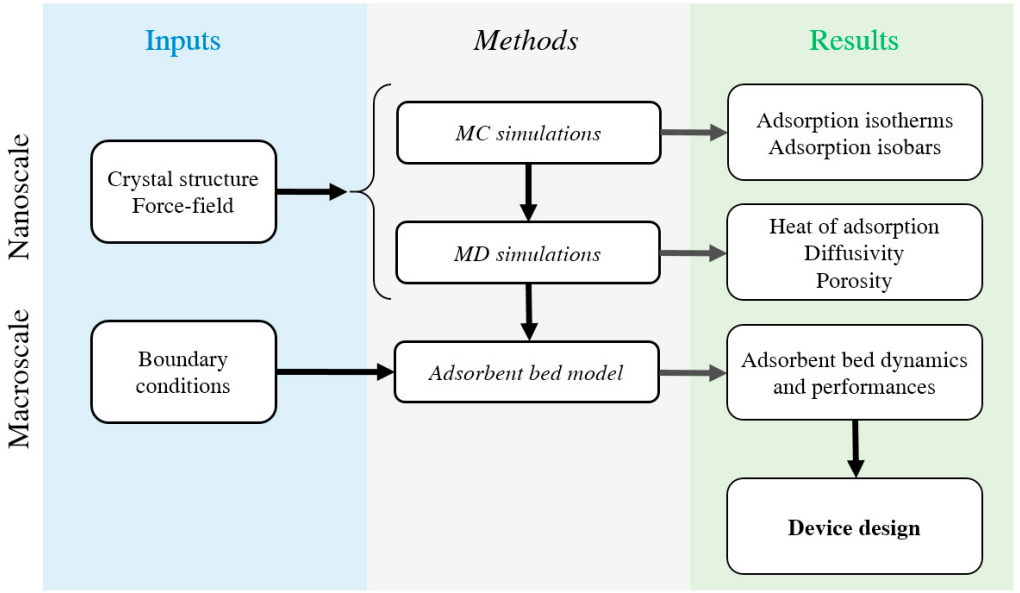

Fig. 6. Schematic of a multiscale simulation approach to design sorption heat storage devices, starting from adsorbent materials with heat and mass transfer properties not yet characterized.

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