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REVIEW

Adsorption onto zeolites: molecular perspective

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Abstract

2D minerals are among key elements of advanced systems, but the need for understanding their interactions/reactions with materials and systems in which they are involved necessitates tracking their molecular and atomic monitoring. Zeolitic structures are microporous materials formed in the nature through volcanic activities or synthesis. Because of their outstanding physicochemical properties like cation exchange capacity and excellent adsorption properties, zeolites have found application in diverse chemical processes, e.g., gas adsorption, water purification, and wastewater treatment. Prediction of zeolite performance for a targeted application saves time and expense as such projection could lead to the synthesis of optimum zeolite with adjusted properties. This review paper aims at encapsulating the latest findings on the use of 2D zeolite adsorbents studying three eminent molecular simulation techniques, namely molecular dynamics simulation, density functional theory, and Monte Carlo. Zeolites with precision structures and cost-efficiency for adsorption together with their adsorption capacity were correspondingly discussed in this review. Information gleaned from published reports on simulating zeolites' adsorption properties could bridge with a brief comparison between the techniques mentioned to pave the way for scientists and industries to find the ideal method to predict zeolites performance and select the appropriate zeolite structure for the on-demand application.

Keywords Zeolite · Simulation · Molecular dynamics simulation · Density functional theory · Monte Carlo

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Introduction

Zeolites, hydrated aluminosilicates of alkali elements such as Na and K and other elements like Ca, Li, and Mg, are mainly known as crystalline microporous materials obtained either naturally or synthetically (Bacakova et al. 2018; Servatan et al. 2020a, 2018). Zeolites are comprised of TO_4 tetrahedral blocks that T (usually Si, Al, P) in the center is surrounded by four oxygen atoms, as depicted in Fig. 1 (Vinaches et al. 2017; Yazdi et al. 2020; Khalili et al. 2020; Servatan et al. 2020b). Such tetrahedral forms various types like 6-rings, 8-rings, or 12-rings as a secondary building unit of assorted cages or cylinders, which create a pore network in the zeolite crystal; ~ 250 different forms were produced, with similar chemical composition but different pore topologies (Fig. 1). Such pores are available from the outside, and such materials' exceptional stability makes them ideal candidates for numerous applications (Beerdsen et al. 2006).

Equation (1) shows the chemical composition of the hydrated zeolite (Drioli and Giorno 2016):

$$\left|M_{x/n}\left(\mathrm{H_2O}\right)_Z\right|\left[\left(AlO_2\right)_x\left(SiO_2\right)_y\right] \qquad (1)$$

In this formula, *M* is an extra-framework cation with *n* valence, the molar concentrations of *Al* and *Si* in the zeolite framework are stated by *x, y,* while *z* is the molar concentration of H_2O. In the conventional building block of zeolite, *T* mainly denotes Al and Si, while in synthetic forms, the *M* element in Eq. (1) could be Na, K, or other cations from the periodic table of elements such as Li, Ca, and Ba (Byrappa and Yoshimura 2001). Zeolites of AlO_4 or SiO_4 possess an anionic structure. The cations in the channels are simply exchangeable, while Al or Si is not exchangeable under usual conditions.

The aluminum's distribution in the zeolite framework generally obeys two rules: Loewenstein's rule and Dempsey's rule. Loewenstein's rule states that no framework Al-O-Al linkages exist among the zeolites (Loewenstein 1954). According to the Dempsey's rule, between two Al atoms of the structure of the zeolites, there must be at least three Si atoms because the presence of Al atoms in a shorter distance is unfavorable in terms of energy (Dempsey et al. 1969). Although there are a significant number of zeolites denying Dempsey's rule, Loewenstein's rule is acceptable for most of the discovered zeolites except a few like heulandite (HEU) zeolites (Slaughter and Yu 1991). Besides their high porosity, in terms of chemical structural position, zeolites are so variable that around 250 different types of zeolites have been identified so far (Mintova et al. 2013). From this perspective, zeolites are categorizable into three major groups: Si/Al ratio ≤ 2, 2 < Si/Al ratio ≤ 5, and Si/Al ratio ≥ 5, known as low silica, medium silica, and high silica, respectively. Furthermore, zeolites can be synthesized using natural elements found in the earth due to their abundance and negligible negative effects on the environment (Alver and Metin 2012). The zeolites formation process in nature, which is mainly the result of a reaction between volcanic ash and water, lasts for thousands of years. However, the synthesis process is shorter in laboratory conditions due to providing elevated pressure and temperature using natural raw materials. These materials mainly include those of silica sources like haolisite (Gualtieri 2001) and kaoline (Biel et al. 2020) as clay minerals, and pumice (Burriesci et al. 1983), diatomites (Garcia et al. 2016), and perlite (Dyer et al. 2004) as volcanic glasses. Zeolites are also synthesizable from the wastes of aluminosilicate materials like rice husk ash (Wang et al. 2020), fly ash (Czuma et al. 2019), paper sludge ash (Wajima et al. 2006), etc. There are different synthesis methods, namely hydrothermal synthesis, molten salt method, alkali activation, microwave-assisted synthesis, fusion method, etc., and the first method (hydrothermal synthesis) is the most commonly applied one (Król 2020). In this method, the Al and Si source components are mixed in the presence of an alkali solution having pH > 8.5. The reaction mixture is heated at an elevated temperature (above 100 °C); it will remain amorphous for a while after rising temperature to the synthesis temperature. The process parameters are then controlled for the formation of the crystalline zeolite, where the amorphous material is gradually replaced by a relatively equal mass of crystalline zeolites (Cundy and Cox 2005). From an economic point of view, using natural wastes for synthesizing zeolites is favorably cost-effective, taking into consideration that the costs of collecting and storing the waste will increase the final production cost to a limited extent. From an environmental point of view, it would significantly help to reduce the amount of natural waste polluting the environment. Moreover, more is that synthetic zeolites are advantageous compared to natural zeolites. Research proves that synthetic zeolites are more favorable in removing radioactive waste (Abdel Moamen et al. 2015), have higher adsorption capacity than natural zeolites especially in adsorbing heavy metal ions (Kozera-Sucharda et al. 2020), and have larger pores, which makes them potential candidates for a range of applications (Bandura et al. 2015; Nizami et al. 2016). For example, synthetic zeolites with big pores have been ideal for cleaning up petroleum spoils (Bandura et al. 2015), and those having large interconnected channels are

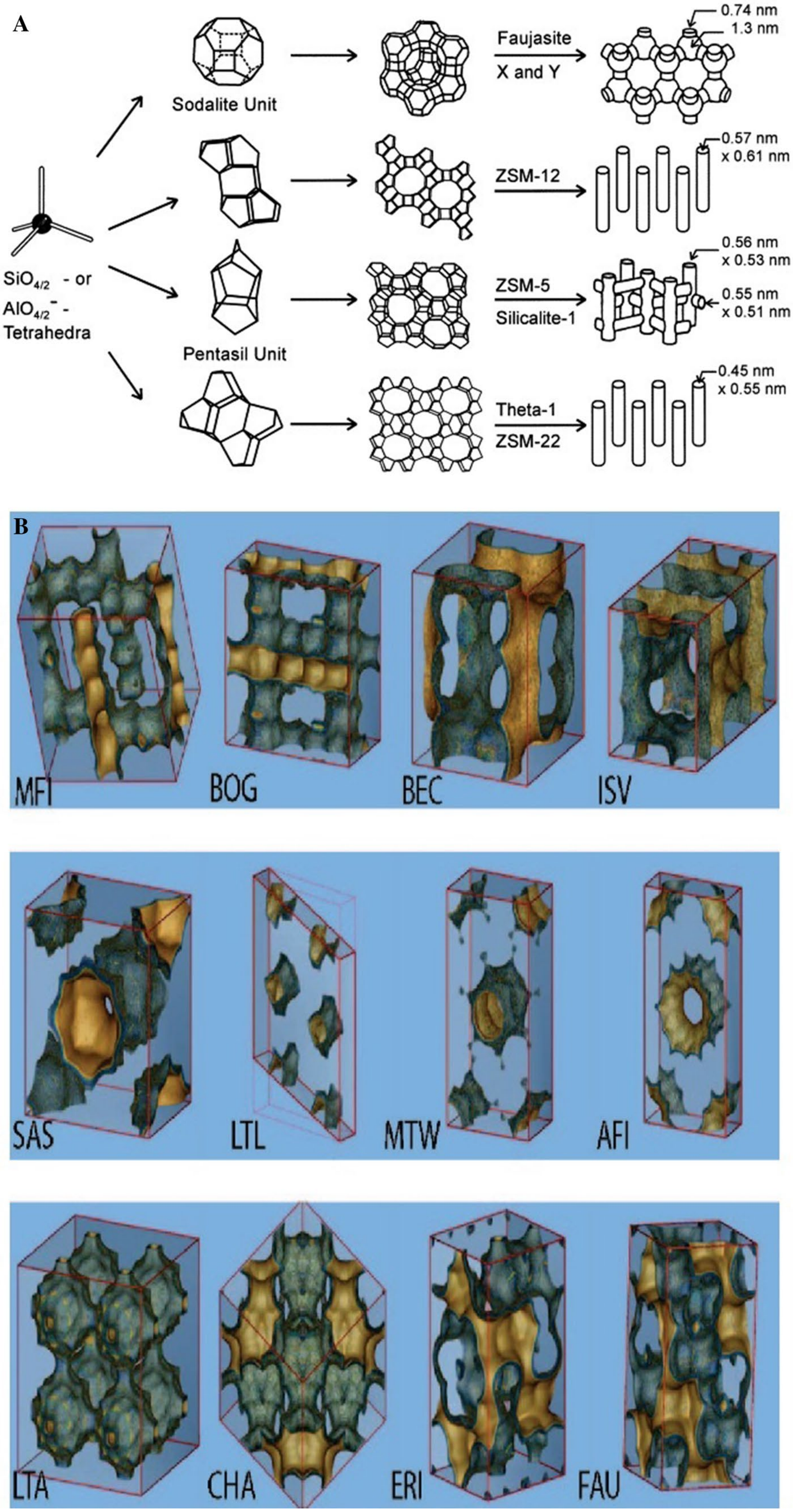


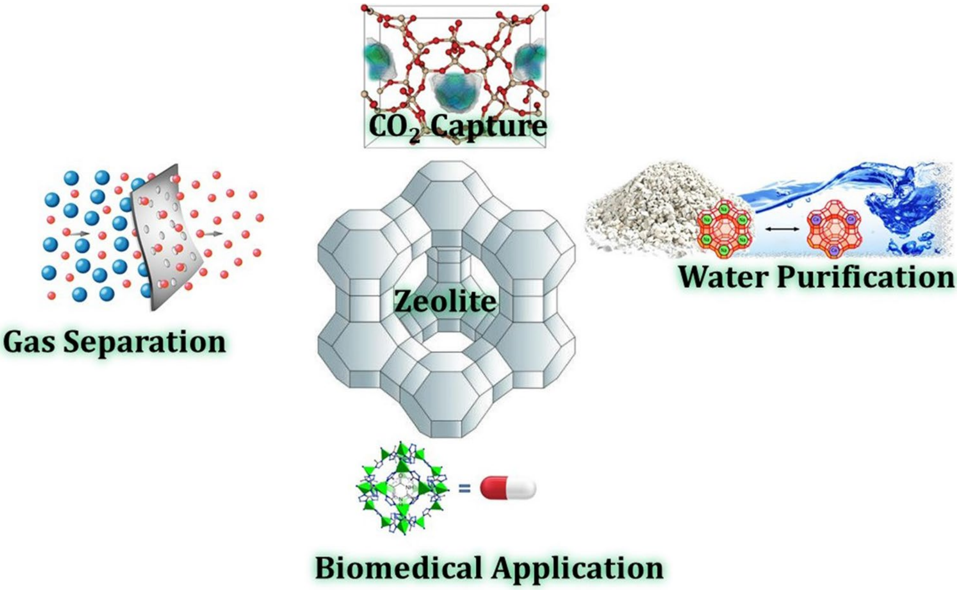
Fig. 1 **a** Structures of four selected zeolites (from top to bottom: faujasite or zeolites X, Y; zeolite ZSM-12; zeolite ZSM-5 or silicalite-1; zeolite Theta-1 or ZSM-22) and their micropore systems and dimensions. Reprinted with permission from (Weitkamp 2000). **b** Examples of some zeolite structures: three-dimensional networks (top), one-dimensional channels (middle), and cage-like structures (bottom) reprinted with permission from (Beerdsen et al. 2006)

more suitable for use as catalysts as they remain stable for a longer time compared to zeolites with smaller pore sizes (Nizami et al. 2016).

Adsorption is a chemical process by which the capability of a porous material in adsorbing one or more components within a gas or liquid flow is measured (Mashhadzadeh et al. 2016; Hamed Mashhadzadeh et al. 2018a, b; Ghorbanzadeh Ahangari and Hamed Mashhadzadeh 2020; Shahmoradi et al. 2020a,b; Karami et al. 2021a). In this process, a liquid or gas mixture is exposed to a porous material, and the separation process is carried out according to the affinity of different components within the mixture toward the porous material. Diverse industries apply the adsorption process such as the dehumidification of the air, water purification (Mahmodi et al. 2020a; Vatanpour et al. 2021), wastewater treatment (Karami et al. 2021b), gas separation like CO_2 capturing, ion exchange, and catalysis (Fig. 2) (Sargazi et al. 2019; Treybal 1980). There have also been some other medicine and drug delivery applications, which have been comprehensively reviewed (Zarrintaj et al. 2020; Mahmodi et al. 2020b; Rahmati et al. 2020). One of the critical parameters for the adsorption process is selecting the appropriate porous material as the adsorbent (Bhattacharya et al. 2008). Several parameters have to be considered for this material, such as porosity, cost-efficiency, abundance, and ease of operation. Given the properties of zeolites, these materials are considered potential adsorbents.

It is necessary to have access to the adsorbents' equilibrium data to design the equipment required for the industry's adsorption process properly. The first data needed are the adsorption isotherm indicating the amount of the materials adsorbed by a specific amount of the applied adsorbent. The second is the heat of adsorption, indicative of the release of heat caused by the materials' adsorption by a certain amount of the adsorbent (Calleja et al. 1998). Nevertheless, experimental methods may encounter some difficulties and restraints as there might be limitations to conduct the experiments in a particular range of operating conditions such as temperature and pressure due to the restricted capability of the experimental apparatus deployed (Rahmati and Modarress 2009a), or the method itself could be less cost-efficient. Therefore, to identify or substitute experimental methods with comparatively useful and accurate procedures, some theoretical models were improved to predict the adsorption process onto adsorbents, namely Langmuir, BET isotherms, and Kelvin equation (Sweatman and Quirke 2001; Lima et al. 2021). However, they were not sufficiently efficient and displayed limitations in predicting the adsorption process under some situations (Ungerer et al. 2005). Molecular simulation techniques have been developed as efficient, accurate, and expeditious methods to obtain the isotherms of adsorption (Tassel et al. 1991; Bates et al. 1996; Pillai et al. 2012), owing to modern statistical thermodynamics improvements. Density functional theory (DFT) (Hoffman et al. 2019; Salmankhani et al. 2020), Monte Carlo (MC) (Smit and Krishna 2001; Khorasani et al. 2014), and molecular dynamics simulation (MD) (Demontis et al. 2010; Khadem et al. 2021) are the most popular molecular simulation techniques which have been contributing to the science of zeolites. In this regard, enormous progress has been achieved with expanded accuracy, increased complexity, and improved integrity of modeling techniques. It is noteworthy to mention that MC and DFT are mainly applied to model zeolite structures and study their behavior while MD is used to investigate their mechanism of the process and to observe how molecules move through each other. Although

Fig. 2 The main zeolite applications in different fields, including CO_2 capture, gas separation, biomedical application, and water treatment



the number of theoretical articles regarding zeolite structures has fluctuated over the last two decades, the future for the modeling techniques in zeolites industries is bright.

In scientific terms, zeolites are intriguing and challenging due to the activity inside the material, and molecular interactions are difficult to predict; thus, it is tough to perform experiments to achieve data at the level of molecules. Evaluating the pores' interaction or reaction requires cognizance about the reactants' adsorption, molecular diffusion, a chemical transition to an active site, and the products' desorption from the active zeolite site. These steps could have an influence on the rates of reaction and in the formation of the products. It is more difficult to obtain information at the molecular level of the molecules of interest inside the material. Concerning this feature, the molecular simulations support the experiments for obtaining an accurate interpretation of the results. Herein, we have endeavored to provide a comprehensive overview of the importance of molecular simulation techniques' in investigating the adsorption process using zeolites as adsorbents. The next section briefly explains the MD, followed by a discussion on the MD-based literature investigating zeolites' adsorption process. Afterward, the philosophy of introducing the DFT method is expounded with the relevant literature simulating the adsorption process in zeolites using the DFT technique. Subsequently, the Monte Carlo method is discussed, and finally, the importance of these simulating techniques soon is deliberated.

Molecular dynamics (MD) simulation

The methodology of MD

The molecular dynamics simulation technique is based on the fundamental premise that every substance comprises atoms and molecules and the motion of the molecules is determined by the second Newton's law (Abdelrasoul et al. 2017; Mohammadi et al. 2018; Saeb et al. 2015,2016). Furthermore, while a molecule moves within the studied system, other molecules in its surroundings might interact with it and exert different forces on the molecule, namely van der Waals force. As a result, to consider these significant interactions, force fields should be applied (Hussain and Titiloye 2005). Therefore, selecting the proper force field for the system under consideration and/or the development of an appropriate force field is the most challenging issue to predict the desired properties accurately. Another important point to consider is the time step of applying the force. Time step has to be very short to enhance the accuracy of the simulation and track the continuous movement of the molecule (such as 10^{-15} s). The forces exerted on each molecule are calculated during every time step. According to the forces and the velocity of each molecule at the current time, the local situation and the velocity of the molecule are predictable for the next time step. As time step is primarily short, it can be assumed that the forces exerted on each molecule are constant. Consequently, the movements of the molecules within the system are analyzed, and their local situation for the next time steps is obtained. Since the physical properties of every substances, such as temperature, are dependent on its molecules' behavior, determining the molecules' motion pattern leads to ascertaining the amount of the physical property of the substance (Maroo and Chung 2008). Moreover, the thermodynamic properties of every material are dependent on the movement of its atoms and molecules. Thus, the mentioned properties are obtainable after obtaining the behavior of the molecules of a system only. The structural simplicity of MD simulation compared to methods including atomic level interactions such as electrons and orbital has made it a favorable simulation technique for worldwide use. Nevertheless, this simulation technique brings about some limitations for selecting an appropriate force field among the existing ones or developing a new one as already stated. Furthermore, another issue restricting the applications of MD simulation is the CPU time.

Applications of MD

The uniform internal surface area of zeolites allows them to accomplish chemical transformations through their channels, thus enabling them to absorb, separate, and remove gases, hydrocarbons, and contaminants under different environments. Besides, introducing mesoporous channels to microporous structures has recently been an effective route to improve their diffusivity (Bai et al. 2016). Bai et al. (Bai et al. 2016) modeled a hierarchical SSP zeolite system, including MFI microporous zeolite and mesoporous channels, to probe cyclohexane diffusion under molecular dynamics simulation (MD). Using the GROMACS package and Einstein relation, they measured diffusion in this type of zeolite depending on motions in microporous regions. At higher temperatures only, mesoporous channels can sufficiently populate, and the diffusion exceeds that of conventional microporous zeolite. It has been shown that large free energies for escaping from the micro- to mesoporous region result in unusual transport behavior. Arya et al. carried out an MD-based study to investigate the effect of pore exit on the transportation of CH_4 molecules through $ALPO_4{}^{-5}$ pores (Arya et al. 2001). They reported more surface barrier effects of pores at lower sorbate loadings even though they were less affected by other sorbents' presence; their model

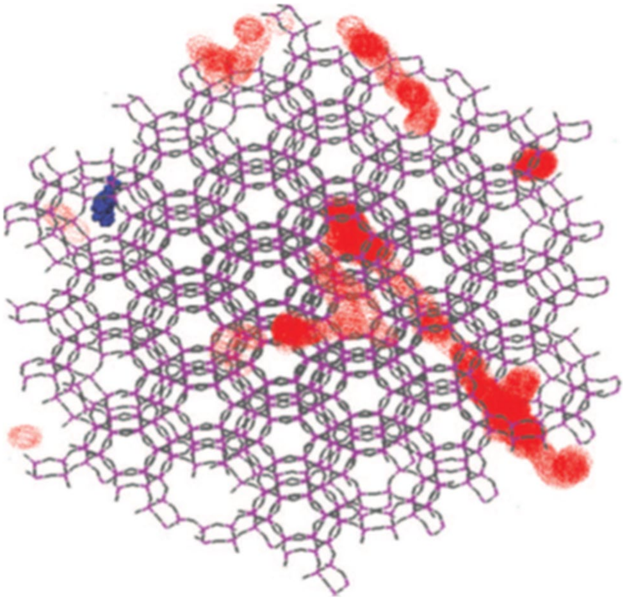
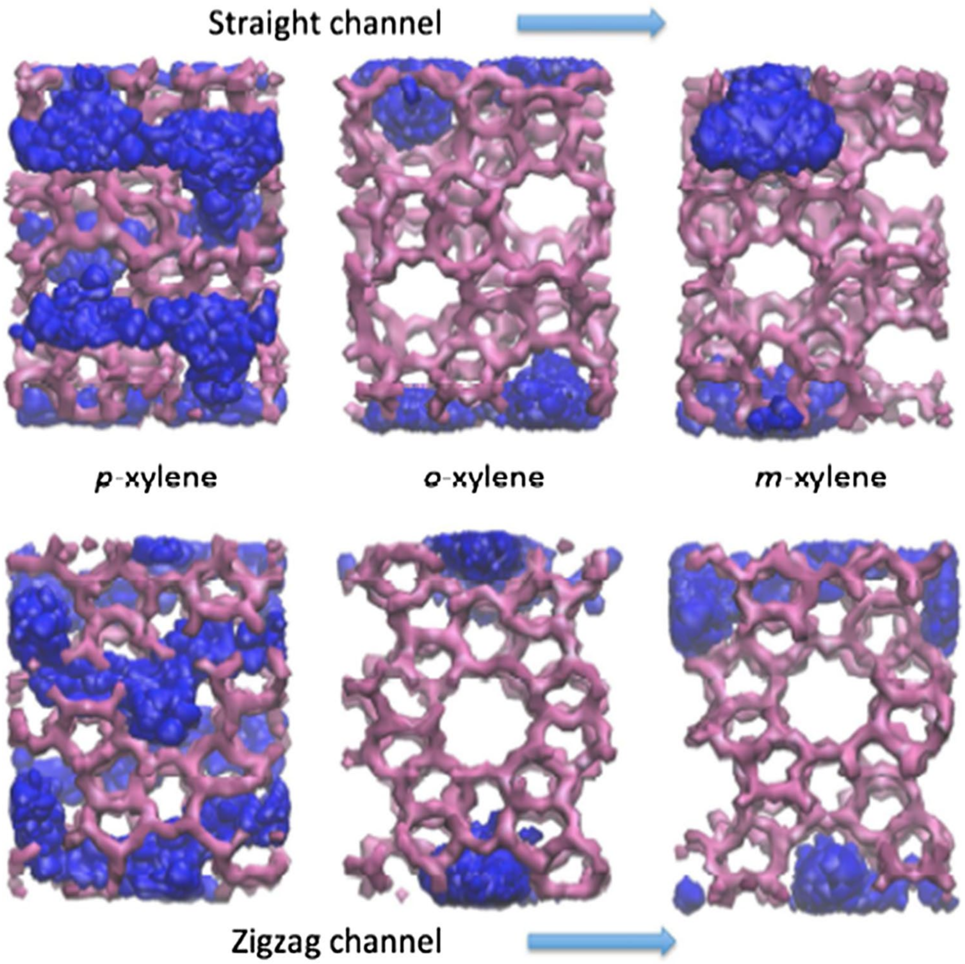


Fig. 3 Diffusion of *n*-pentane (blue, dark in black and white) and neopentane (red, gray) within NaY framework obtained from MD simulations at 200 K Ref. (Borah et al. 2010)

could correctly predict the exit barrier effects as a function of temperature. Bora et al. used both MD simulations and quasielastic neutron scattering (QENS) to predict the diffusion of neopentane, isopentane, and n-pentane in NaY zeolite (Borah et al. 2010). Their results revealed higher self-diffusivity of iso- and neopentane compared to n-pentane at 300 K and higher activation energy (Ea) of *n*-pentane in contrast, (Ea(*n*-pentane) > Ea(isopentane) > Ea(neopentane)). Furthermore, their MD simulation showed existing energetic barriers at the bottleneck of *n*-pentane, while no such barriers were observed for the other two isomers. Figure 3 presents the pathway of different isomers through NaY zeolite provided by Bora et al.

In another MD study, Bu et al. considered the diffusivity of various biomass pyrolysis vapors, including water, glycolaldehyde, methanol, and toluene and representative biofuel molecules, namely xylene isomers in H-ZSM-5 zeolite (Bu et al. 2017). They proved a good agreement of their results for the diffusion of biomass pyrolysis vapors compared to available NMR measures and the importance of molecular orientation on diffusivity. Furthermore, xylene isomers' results revealed that the *p*-xylene molecule could diffuse

Fig. 4 Switching trajectory of *p*-xylene between channels against the trajectory of the *o*- and *m*-xylene only through the original channels Ref. (Bu et al. 2017)



along both zigzag and straight channels, while the *o*-xylene and the *m*-xylene were not able to switch between due to lower diffusion as depicted in Fig. 4.

Adsorption of methane using Si-LTA zeolite was investigated by Combariza et al. under the MD framework (Combariza and Sastre 2011). Using energy profiles, 2D occupational densities, and the adsorption process along the z-direction, they could show the preferential zones of interaction, according to van der Waals interactions. Moreover, they revealed an increase in surface permeability as a function of loading using both the MD results and Schuring's analytical equation. CO_2 adsorption on the modified AU NaY siliceous, Na88(SiO4)44, zeolite by sodium dodecyl sulfate surfactant (SDS) was investigated by Ortega et al. (Valencia-Ortega et al. 2019), where the principle adsorption of CO_2 was due to the free ions in the zeolite. Since the sodium ions are mainly deposited close to the surface, adsorption occurred near the surface. In the absence of surfactant, zeolite could not adsorb all the CO_2 itself, and its adsorption capacity decreased. The simulation results elucidated that in the absence of a surfactant, zeolite could partially adsorb the CO_2 even in a highly populated CO_2 atmosphere. A similar trend was the case for zeolite surfaces rich in surfactant, while at an optimal amount of CO_2 complete adsorption was gained. It is concluded that CO_2 adsorption onto zeolite is improved by surface modification using a surfactant at low CO_2 concentrations. A summary of MD-based articles regarding the adsorption/diffusion properties of zeolites is provided in Table. 1.

Besides the applications above, zeolites can be considered a significant candidate for water purification and water treatment due to their advantages over conventional treatment processes such as reverse osmosis (RO) (Shannon et al. 2010; Gupta et al. 2016). Accordingly, the zeolites' influences have been investigated on the water treatment processes in the last few years, both theoretically and experimentally. Cohen et al. modeled an LTA-type zeolite membrane capped with hydrophobic and hydrophilic moieties by MD simulations to evaluate the water transport under varying pressure of 50–400 MPa (Turgman-Cohen et al. 2013). A 15 ns monitoring of simulation showed a higher water adsorption rate on the membrane's surface for the hydrophilic membrane. Water flux was independent of the pressure drop in both types and was also lower than the bulk form membranes of the same zeolite. The authors also proposed that applying a periodic pressure difference between the inlet and outlet could direct the water to flow toward the low-pressure cages. Mousavi et al. used MFI zeolite nanosheets to remove chemical contaminants, including mercury chloride ($HgCl_2$) and copper chloride ($CuCl_2$) from water in an MD-based study (Rassoulinejad-Mousavi et al. 2020). They modeled a simulation box including a zeolite membrane and a mixture of the hazardous elements with water, as shown in Fig. 5. MFI zeolite could effectively confine mercury, copper, and chlorine permeation ions without affecting water flux rate and employing non-equilibrium MD simulations. Jamali et al. considered the salt separation capacity of 27 types of zeolites (Jamali et al. 2017) by modeling zeolites with orthorhombic unit cells and the pore-limit diameters (PLDs) of more than 2.8 Å (the minimum diameter of water molecules). They established that the zeolites with PLDs smaller than 5.5 Å would show higher separation properties, while those with greater PLDs must be more adjudicated in terms of their channels shape or cross-sectional area.

Hu et al. selected ZIF-8 zeolite to model new RO membranes for water purification using MD simulations (Hu et al. 2011). They selected this type of zeolite due to its high thermal and chemical stability and high mechanical strength, making it strong enough to withstand high external pressures during the desalination process. The designed membrane successfully rejects Na + and CL^- ions, while it did not confine water flux. Their proposed membrane also showed strong fouling resistance and large water permeation. In a combined MD-experimental article, Nagar et al. designed a novel membrane of zeolite MFI/hydrophobic polyvinylchloride (PVC) matrix to purify kitchen wastewater using microbial fuel cell (MFC)-based treatment method as shown in the schematic of Fig. 6 (Nagar et al. 2019).

MD was used to model the zeolite/PVC, pristine PVC, and Nafion membranes, which indicated that the zeolite membrane had high ion exchange capability and water sorption and is a better membrane for wastewater treatment compared to pristine PVC or Nafion membranes. Their experimental results also demonstrated a considerably lower cost of producing this membrane than the Nafion type (3$ against 7$). The exciting outcomes obtained from molecular dynamics investigation of zeolites in the context of water purification applications widened the horizons of using zeolite materials for developing water treatment membranes.

In conclusion, we can see that a wide variety of zeolites, especially those having Si^{4+} and Al^{3+} in their structure, together with different pollutants due to providing distinctive electrostatic and van der Waals forces, have been considered in atomic and molecular simulations. The simulation could provide very high pressures as high as 500 MPa, which are not obtainable in the laboratory. Various factors such as water flux, radial distribution function (RDF), mean squared displacement (MSD), and water and ions density have been predicted to give valuable insights into its effects on zeolite structure and pollutants for experimental analyzes. The inherent simplicity of the molecular dynamics

Table 1 Adsorption/diffusion properties of zeolites from molecular dynamics studies

No.	Zeolite type	Adsorption/diffusion element	Main findings	Ref
1	FAU (NaY)	Pentane isomers	Higher diffusivity of iso- and neopentane than *n*-pentane while the activation energy of *n*-pentane was higher than the other two	Borah et al. (2010)
2	Si-LTA	Methane	Higher CH_4 permeability as a function of loading	Combariza and Sastre (2011)
3	AU NaY siliceous, Na88(SiO4)44	CO_2	Higher adsorption of CO_2 by using SDS surfactant on the zeolite	Valencia-Ortega et al. (2019)
4	Zeolite silicate	Alkane chains (n-C8 and *n*-C16)	The higher diffusion coefficient for both alkanes compared to experimental data. Switching between channels was observed at higher temperatures	O'Malley and Catlow (2013)
5	ZSM-5	Ethanol	Excellent vibrational density. Obtained adsorption energy by MD was closer to experiment reports compared to those obtained by the traditional harmonic frequency method	Alexopoulos et al. (2016)
6	SOF, STW, ITQ-37	CHBrClF and 4-ethyl-4-methyl octane isomers	STW was enantioselective for both isomers, unlike SOF or ITQ-37. Adsorption selectivity depended only on pore geometry, not by the Ge substitution. ITQ-37 showed selectivity when it was shrunk by 30%	Castillo et al. (2010)
7	Chabazite	Water	Self-diffusion was possible at 300 K. at high loading and temperatures, long term electrostatic interactions affected the self-diffusivity	Chanajaree et al. (2011)
8	HSAPO-34	Water/methanol	Upon increasing the amount of water or methanol adsorbed, the zeolite framework could expand or shrink. The proton mobility observed proton affinity of adsorbates, mobility of guest molecules, and the load volume of adsorbates	Wispelaere et al. (2015)
9	ZSM-5	*n*-Dodecane (*n*-C12), benzothiophene (BZT)	BZT showed better self-diffusivity than *n*-C12 at all temperatures. Self-diffusivity increased for both as a function of temperature	Ferreira et al. (2016)
10	a series of 8-ring zeolites	Ethene/propene	Ethene diffused easier than propene. Diffusion of ethene is an activated process depending on the acidity, temperature, and topology of zeolite	Ghysels et al. (2015)
11	Zeolite 3A	Water/CO_2	CO_2 and water compete for adsorption on 3A, and lower temperatures are needed for selective removal of water	Jafari et al. (2020)

Table 1 (continued)

No.	Zeolite type	Adsorption/diffusion element	Main findings	Ref
12	FAU	*n*-hexane and 2,2-dimethyl butane	Self-diffusivity depends on the hexane diameter so that 2,2-dimethyl butane with the largest diameter has the largest D_s. The activation energies, E_a, for the branched isomers were lower than that for nC_6	Thomas and Subramanian (2017)
13	BEA	*n*-hexane and 2,2-dimethyl butane	Changes in diffusivities and activation energies between single crystal and 'powder' sample dependence on the nature of the zeolite sample as well as the type of guest molecule	Thomas and Subramanian (2019)

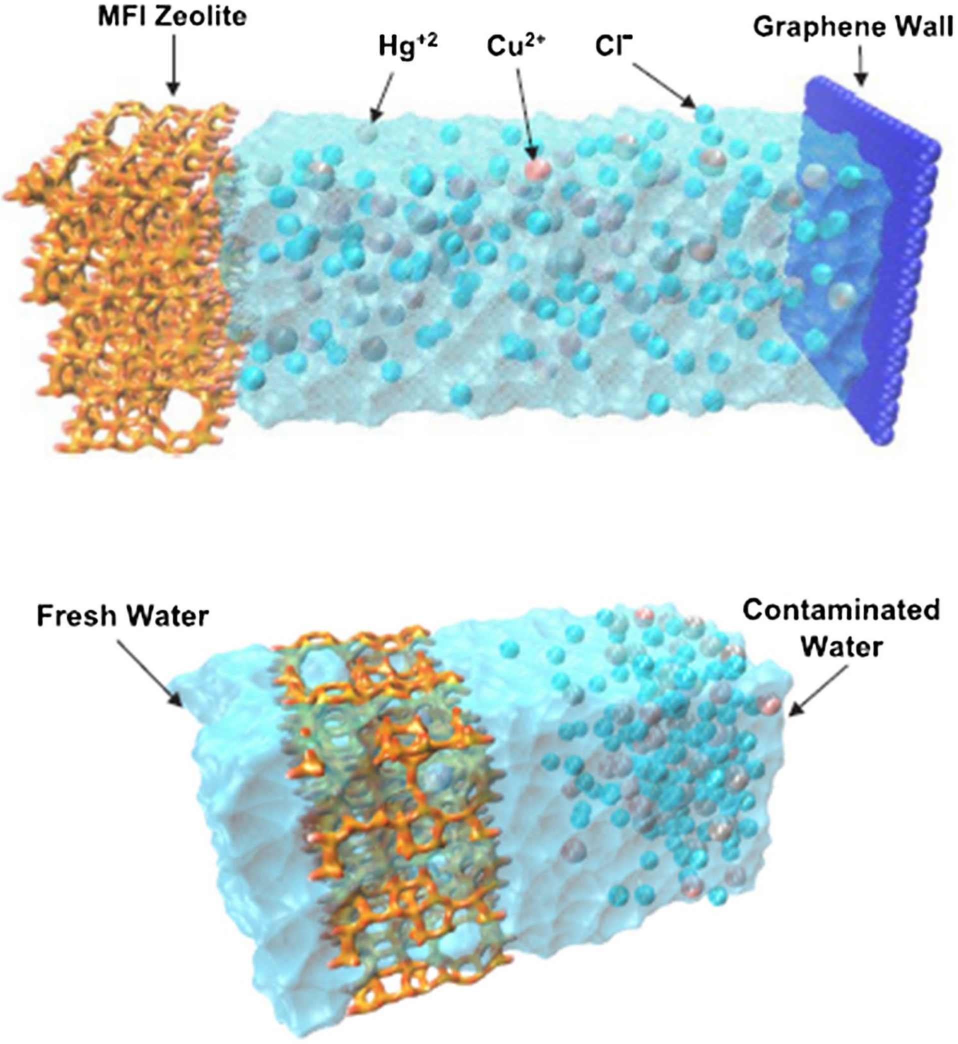


Fig. 5 Schematic of the simulation box including MFI zeolite and contaminated water Ref. (Rassoulinejad-Mousavi et al. 2020)

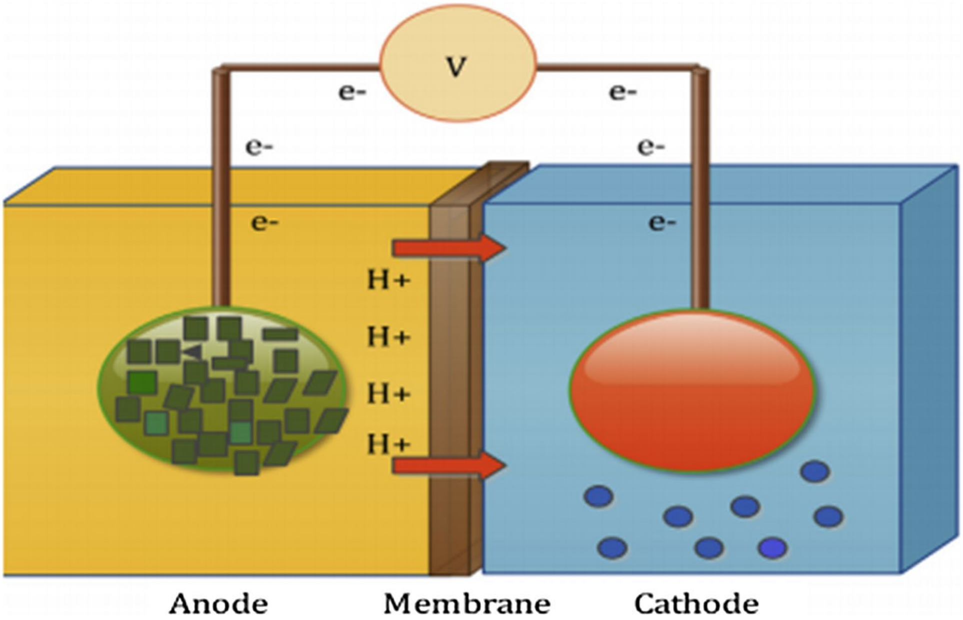


Fig. 6 Schematic for the MFC setup, including zeolite/PVC membrane in the middle for kitchen wastewater treatment (Nagar et al. 2019)

simulation due to the lack of electrons and orbitals as well as its fast character due to the use of fewer equations have been the main reasons for its worldwide use (Laaksonen and Tu 1999).

Density functional theory (DFT)

The methodology of DFT

Quantum mechanics (QM) has been developed to describe electrons and individual molecules' behavior, which cannot be carried out using classical mechanics. Schrodinger equation, the central equation of QM, describes electrons' behaviors within the atoms and molecules (Nakatsuji et al. 2007).

$$H\Psi = E\Psi \tag{2}$$

where H is the Hamiltonian operator, E is the energy, and Ψ is the wave function. Ψ describes the electron based on probability, so it does not show the exact position of electrons in the atoms and molecules yet show how probable it is to find the electron somewhere. In general, the following equation describes the H parameter in the Schrodinger equation (Abdelrasoul et al. 2017):

$$H = -\sum_i \frac{h^2}{4\pi m_e}\nabla_i^2 - \sum_k \frac{h^2}{4\pi m_k}\nabla_k^2 - \sum_i \sum_k \frac{e^2 Z_k}{r_{ik}} + \sum_{i<j} \frac{e^2}{r_{ij}} + \sum_{k<l} \frac{e^2 Z_k Z_l}{r_{kl}} \tag{3}$$

where i and j are electron counters, and k and l are nuclei counters. h is Planck's constant, m_e and m_k are the masses of electrons and nuclei, respectively, r is the distance between two particles, e is the charge of the electron, Z is the atomic number of nuclei, and ∇ is the Laplacian operator. The first and second terms of the above equation indicate the kinetic energy of the electrons and nuclei. The rest of the terms represent the electric potential energy of the electrons and nuclei. The complexity of the equation, as mentioned above, can be reduced using the Born–Oppenheimer approximation. According to this approximation, the nuclei's mass is so high that they move very slowly when they have exerted an equal force on the electrons. Thereby, one can assume that the nuclei are static. Therefore, it can be stated that the Schrodinger equation contains variables dealing with electrons. Although the Schrodinger equation can theoretically predict atoms and molecules' properties, it can be solved analytically for the atoms with only one electron, such as H, He^+, Li^{2+}, and C^{+5} in practical terms. Different solutions have been suggested, such as density functional theory (DFT), to enable the Schrodinger equation to investigate other atoms and molecules. This technique adapted from the Hohenberg-Cohen theorem expounds that an atom or molecule's energy can be calculated via electron density instead of Ψ. The number of electrons and the atomic number of atoms are obtainable using electron density. Subsequently, this information can be applied to calculate the Hamiltonian operator and to calculate the Schrodinger equation. Since DFT considers the atoms' electrons, it is expected that the data acquired using this method are comparatively accurate. On

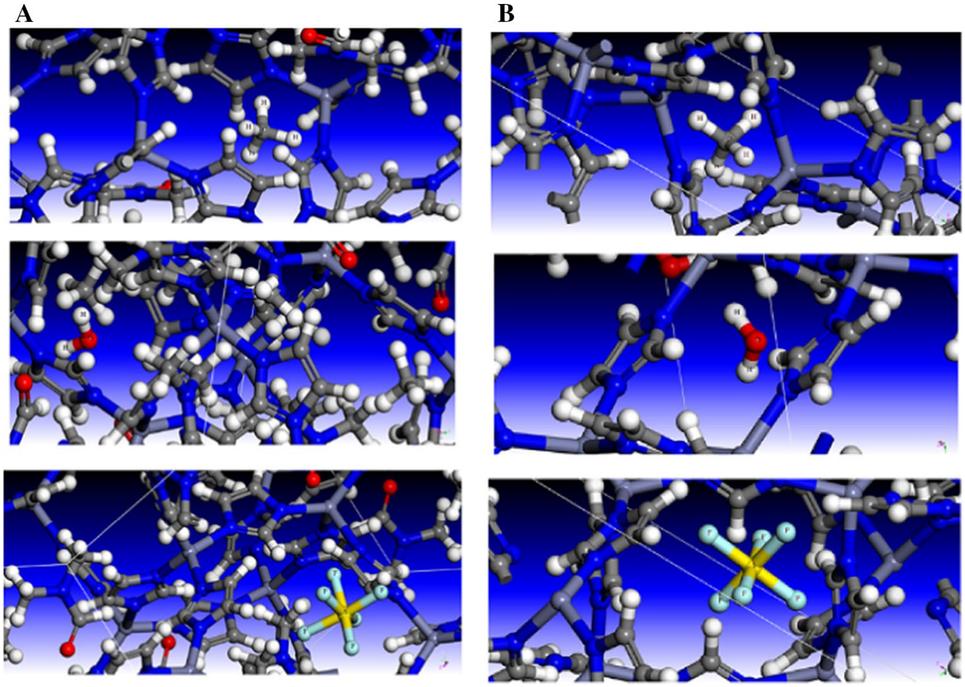


Fig. 7 The binding sites of SF_6, CH_4, and H_2O in **a** ZIF-4 and **b** ZIF-6 Ref. (Bensiradj et al. 2019)

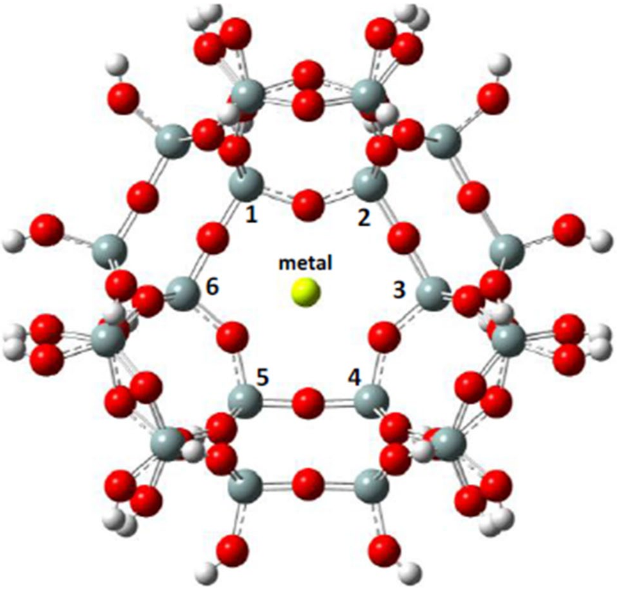


Fig. 8 Schematic for a 24 T ERI zeolite modeled using DFT with the location of Ca, Mg, and Be metal atoms on 6 T membered ring Ref. (Fellah 2017)

the other hand, the calculations carried out via this method are heavier and more complex than MD. Consequently, for systems including high numbers of atoms, the DFT method is not cost-efficient.

The applications of DFT

Researchers have used the DFT technique to investigate zeolites' adsorption processes in many research studies for MD. In this regard, Bensiradj et al. applied DFT to consider the adsorption properties of ZIF-4 and ZIf-6 toward SF_6, CH_4, and H_2O. They considered different binding sites, as shown in Fig. 7, and reported that the co-adsorption of three gases was impossible due to the unavailability of enough pore space. The capture of the gases individually was favored in ZIF-6, and the maximum adsorbed content of CH_4 was observed in the same zeolite at high pressure (Bensiradj et al. 2019).

Ag and Cu ion-exchanged faujasites have been used in a combined DFT-experimental study provided by Kumar et al. to remove H_2S from dilute streams including He, N_2, CO_2, CO, and H_2O (Ungerer et al. 2005). Ag–X and Ag–Y could

Table 2 Adsorption/diffusion properties of zeolites from DFT studies

No.	Zeolite type	Adsorption/diffusion element	Main findings	Refs
1	Mg-ERI, Ca-ERI	H_2	The released energy for the adsorption of H_2 in the studied zeolites is larger than the enthalpy of liquefaction of H_2 molecules, indicating that these zeolites can be considered potential candidates for hydrogen storage	Fellah (2017)
2	Ag and Cu modified faujasites	CO, H_2O, H_2S, N_2, and CO_2	Ag faujasites zeolites have a high capacity for separating H_2S in the mixture of other species. Although Cu faujasites zeolites can remove H_2S from the mixture containing N_2, H_2O, and CO_2, it cannot remove this gas in the presence of CO	(Kumar et al. (2011))
3	Cation-exchanged SAPO-34	C_2H_6, C_2H_4, C_3H_8, C_3H_6	The affinity of Mg-SAPO-34 toward alkenes is higher than toward alkanes. The nature of exchanged cations does not have a significant effect on the adsorption of the alkanes	Fischer and Bell (2014)
4	ZIF-1, ZIF-4, ZIF-6	H_2O, CO_2	The zeolites adsorb H_2O more selectively than CO_2. The agreement between simulated and experimental results is excellent	Timón et al. (2015)
5	H-ZSM-5	C1-C4 primary alcohols	The released energy of chemisorption of the alcohols increases as the carbon number increases. The probability of the adsorption of the alcohols in zigzag channels is more than in straight channels	Nguyen et al. (2010)
6	NaY	CO_2,N_2,CH_4,C_2H_6, and SF_6	Owing to the strong make the strongest adsorption complex by N_2, the permeation of other gases increases. As a result, the selectivity enhances	Chatterjee and Iwasaki (1999)
7	Ag-MOR	I_2	The more the Ag content is, the stronger the adsorption of I_2 is. The less the ratio of Si/Al is, the more the capacity of the adsorption of I_2 is	Jabraoui et al. (2019)
8	ZIF-4, ZIF-6	SF_6, CH_4, H_2O	In terms of thermodynamic, the co-adsorption of three gases is impossible due to enough pore space's unavailability. The maximum adsorbed content of CH_4 is observed in ZIF-6 at high pressure. The binding sites of the three gases in the studied zeolites are shown in Fig. 7	Bensiradj et al. (2019)
9	HY, HSZM-5	Mono-branched alkanes	Since HY's pore size is elevated, the confinement effect is less significant than in HSZM-5 zeolite. Therefore, by increasing the length of the mono-branched alkanes' side-chain length, the adsorption's energy increases with a lower slope in HY	Fu et al. (2017)
10	Zn, Co, and Ag modified NaX	H_2S, COS	AgX has the highest capacity for H_2S and COS adsorption. The adsorption between gases and the zeolites caused by the bond between S and the metal, such as the Ag–S bond, is the strongest among other zeolites	Chen et al. (2018)
11	FAU	I_2, CH_3I, CO, H_2O	Ag-FAU and Cu-FAU can be considered as potential candidates for I_2 and CH_3I adsorption. H and Li FAU reduce their efficiency for the adsorption of I_2 in the presence of CO and water	Chebbi et al. (2017)

Table 2 (continued)

No.	Zeolite type	Adsorption/diffusion element	Main findings	Refs
12	NaA, CaA	N_2, O_2	Since the adsorption energy difference of Ca^{+2} is elevated, this ion is better for the gas molecule's separation. The electrostatic interaction between N_2 and exchanged ions is strong	Chandrakumar and Pal (2002)

adsorb H_2S in the presence of all other existing elements, while Cu–X and Cu–Y failed to remove H_2S in the presence of 2% CO (Kumar et al. 2011). In another DFT-based study, Fellah et al. investigated the adsorption of H_2 molecules using Mg-, Ca-, and Be- modified 24 T ERI zeolite clusters as depicted in Fig. 8 (Fellah 2017). Their findings demonstrated higher adsorption energy and better chemical potential for the Be-ERI cluster compared to Mg-ERI or Ca-ERI. However, these two clusters showed better electronegativity and chemical reactivity than Be-ERI. Furthermore, they reported that the hydrogen adsorption enthalpy values for Mg-ERI and Ca-ERI clusters were equal to − 3.6 kJ/mole and − 3.9 kJ/mole, respectively (Fellah 2017). Table. 2 provides a summary of the literature on the adsorption in zeolites using the DFT technique.

In DFT simulation, fewer atoms are considered, which enhances the performance of calculations. For instance, diffusion can be more accurately visualized, leading to a more realistic outcome with a comprehensive image provided for interaction determination. Moreover, functional groups' effect in removing contaminants and their interactions with the sorbent can be detected. On the other hand, considering fewer atoms can be a drawback of these systems, such that results would be of lower reliability for practical cases in which adsorption and removal of contaminants are on a large scale (Aliano et al. 2012; Gomes et al. 2019).

Monte Carlo (MC) simulation

The methodology of MC

MC is yet another technique to determine the arrangement of the molecules in a system. Here, the arrangement of molecules in each configuration is entirely random, dependent on the last configuration, unlike the MD technique by which the motion and the position of the molecules are obtainable using Newton's law. There are several criteria for generating a new configuration from the last one. To find a pattern for determining the distribution of the system's molecules, Metropolis et al. (Metropolis et al. 1953) developed a method through which the distribution of the molecules is determined based on the Boltzmann distribution function. To determine the physical properties of a system via the MC method, the amount of the desired property is calculated for each configuration, and finally, the property is obtained by averaging the amount of the property in all configurations (Abdelrasoul et al. 2017). According to the system simulation using MC, some properties are kept constant to calculate the amounts of others. As a result, the MC technique can be carried out in different ensembles (Papadopoulou et al. 1993). In this section, several of them are briefly explained.

Canonical ensemble MC (CMC)

In this ensemble, temperature (*T*), pressure (*P*), and the number (*N*) of atoms are kept constant. This ensemble provides this opportunity to calculate the system's pressure and other properties using the equation of state (McQuarrie 2000), ensemble being mainly applied for studying single-phase systems.

Isothermal–isobaric canonical MC

In this method, temperature, pressure, and number of atoms are fixed, which is possible by allowing the system to exchange energy with its surrounding. This mode is appropriate to investigate inhomogeneous systems such as phase equilibrium systems. Therefore, this method is appropriate to study adsorption processes (Abdelrasoul et al. 2017).

Grand canonical MC (GCMC)

In the simulation method, the properties of the system are determined while the chemical potential, temperature, and volume are kept constant. Likewise, this method is applied to study inhomogeneous systems such as phase equilibrium systems. Therefore, it can investigate the adsorption process

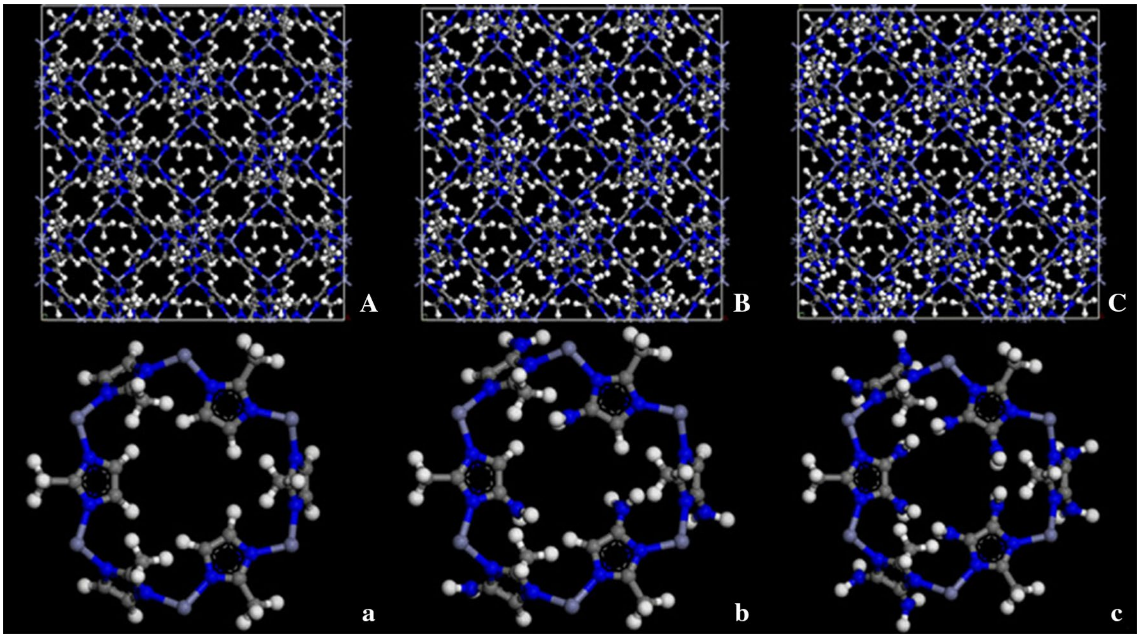


Fig. 9 The crystalline structures of ZIFs modeled by Liu et al. **a** ZIF-8, **b** ZIF-8-NH2, and **c** ZIF-8-(NH2)2 (Zn in purple, C in gray, N in blue, and H in white) Ref. (Liu et al. 2013)

as isothermal–isobaric canonical MC does. In comparison with the last ensemble, this one is more cost-efficient; hence, it is preferable (Abdelrasoul et al. 2017).

The applications of MC

In this section, we have provided a few investigations studying the adsorption process in zeolites using MC. Liu et al. applied GCMC to study the adsorption of CO_2 by ZIF-8, ZIF-8-NH_2, and ZIF-8-$(NH_2)_2$ zeolites as the crystalline structures (Fig. 9) (Liu et al. 2013). Zeolitic imidazolate frameworks (ZIFs) belong to the big family of metal–organic frameworks (MOFs). They are a structure in which Fe, Co, Cu, Zn tetrahedrally coordinated transition metal ions are covalently linked with the aid of imidazolate as a bridging agent Figs. 10 and 11. Their topology resembles zeolite because of the angle between two metal–imidazole bonds with imidazole, which is almost equal to the 145° Si–O–Si angle in the zeolite structure. ZIF-8 is methyl-imidazolate-based zeolite with 1.16 nm cages connected in a hexagonal arrangement appear as the most widely used zeolite in adsorption and storage applications (Phan et al. 2010).

The results indicated that at the low pressure, the order of increasing CO_2 adsorption capacity by zeolites was ZIF-8 < ZIF-8-NH_2 < ZIF-8-$(NH_2)_2$, while at the high pressure, it was: ZIF-8 < ZIF-8-$(NH_2)_2$ < ZIF-8-NH_2. DFT calculations were also applied to calculate CO_2 adsorption sites and binding energies of unmodified and amino-modified ZIF-8, which showed a significant enhancement in the CO_2 adsorption capacity of the amino-functionalized ZIF-8 (Liu et al. 2013). More studies using the MC technique to model and investigate the adsorption process in zeolites are provided in Table 3 (Also see Fig. 11).

Comparing zeolitic structures proves how the interaction between zeolite and a given ion or contaminant occurs and how functional groups improve their adsorption efficiency. So far, a variety of combinations of a contaminant and a zeolite have been theoretically analyzed. Monte Carlo simulation has some advantages, e.g., user-friendly after a relevant computer program has been developed for simulation. Moreover, there are various software commercially developed and available for the MC simulation. Unlike analytical approaches providing closed solutions, a generic Monte Carlo simulation's generic feature is that it is not path dependent and can consider complicated

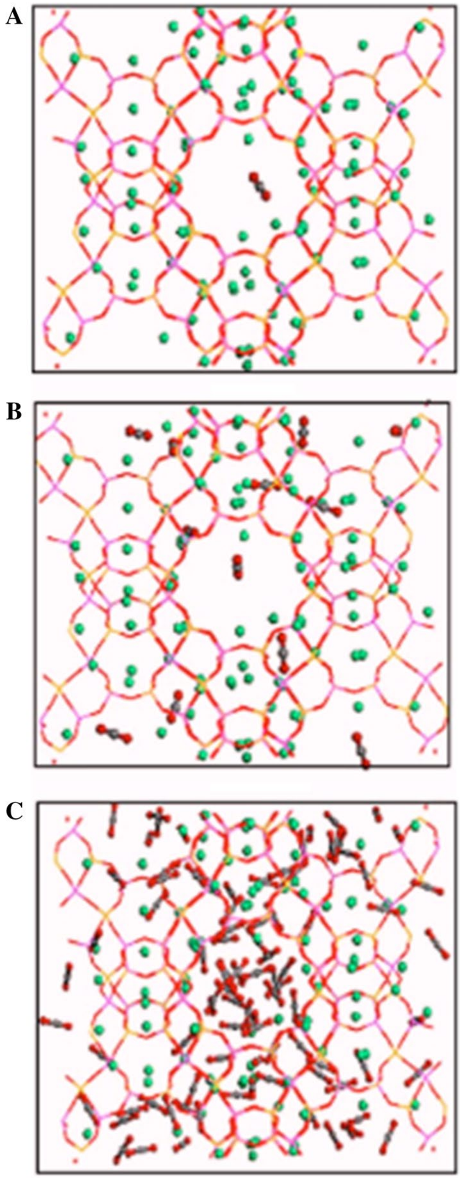


Fig. 10 The amount of CO_2 uptake into NaX zeolite at 305 K and **a** 0.01 **b c** 7.5 MPa (Liu and Yang 2006)

stochastic processes compared with Brownian geometric motion.

Moreover, to a large extent, Monte Carlo simulation methods can be refined to increase the accuracy or reduce the computation time. The Monte Carlo simulation can also identify and provide indicators of the results' accuracy by increasing the number of iterations from generation to generation. On the other hand, there are also some disadvantages of using MC methodologies, e.g., the large number of calculations required. It is also noticeable that in dealing with the limitations of small dimensions, MC appears less efficient than the analytical methods. They are also challenging to understand and often require programming skills (Wu and Buyya 2015).

Conclusion and future perspectives

The first step for the simulation of the adsorption process is choosing an appropriate method among the available techniques explained in this review paper. There would be some reasons behind choosing one technique to carry out the simulation process over another one. For instance, since the MD is dependent on the consumed time, it is possible to estimate the required time for simulation of the adsorption process carried out by MD. On the other hand, it is not possible to estimate the needed time to perform the simulation in the MC technique. Moreover, because MD considers the effect of time, it is possible to simulate the adsorption process as a function of the time. Inevitably, for instance, as mentioned in the main text, MD ignores the influence of the electrons on the adsorption process. Compared to DFT, MD simulation provides the user with an opportunity to simulate the adsorption process in a shorter time interval. Nevertheless, since the DFT method considers more details than the other methods, the results are more precise and trustable and the experimental data can be more closely fit the DFT outcome. Therefore, when accuracy is the matter of concern, DFT would be a preferred method.

It is obligatory to examine the capability of the applied adsorbents for adsorption in order to be able to develop the adsorption process at an industrial scales. Due to the lack of cost-efficiency of the experimental methods, predictive tools such as molecular simulations categorized into different groups, including MD, DFT, and MC, can be interchangeably used to give a more precise picture of the process. It is notable that, in contrast to what an experimentalist may imagine, theoretical simulations are complements to the experimental data. It has been proven that the molecular simulation techniques can bring about profound information about the structure of zeolite adsorbents on a molecular and atomic scale, which is not experimentally possible to detect.

Table 3 Adsorption/diffusion properties of zeolites from Monte Carlo studies

No.	Zeolite type	Adsorption/diffusion element	Main findings	Refs
1	Zeolite 5A	Air	The applied GCMC method can simulate air adsorption into 5A zeolite in quality, yet this simulation has a comparatively high error	Razmus and Hall (1991)
2	Dehydrated zeolite Na-4A	CO_2, N_2, H_2, and their mixtures	The zeolite's selectivity toward CO_2 is high, yet this selectivity gets lower as the pressure increases. In comparison with silicalite, the selectivity of CO_2 is lower on Na-4A	Akten et al. (2003)
3	NaY, NaX, LTA, MFI	H_2S	NaY has been considered the best choice for the H_2S adsorption than other types of zeolites due to higher selectivity	Cosoli et al. (2008)
4	Silicalite-1	Paracresol, water	The energy of the adsorption has an acceptable level of accuracy. In the absence of the paracresol, the adsorption of water into the zeolites is twice higher	Narasimhan et al. (2009)
5	AFR, BOG, LTL	VOCs	BOG is capable of adsorbing a higher amount of VOCs owing to its higher accessible volume. There is a close agreement between the isotherms of adsorption and the Langmuir equation. Zeolites can be considered as a potential candidate for the removal of VOCs	Cosoli et al. (2007)
6	$Ca_{48}X$	H_2	An increment of the pressure leads to a decrement of the capacity of the adsorption. The type of cation in the zeolites framework has an insignificant influence on the simulating hydrogen adsorption. Hydrogen uptake has a strong relationship with the available volume and surface area of the adsorbents	Song and No (2007)
7	ZSM-5	Water	The adsorption capacity enhances as the size of the exchanged cation decreases. The more the Si/Al ratio is, the less the heat of adsorption is	Ding et al. (2008)
8	Zeolite 4A	Propane, propylene	The higher the temperature is, the propane reaches sooner the equilibrium. There is an excellent agreement between the simulation and experimental data in both single adsorption and mixture adsorption	Granato et al. (2007)
9	CHA, DDR, FER, IFR, MFI, MOR, and MWW	H_2S, CH_4	According to the operating condition of the process, MOR and MFI demonstrate higher selectivity toward H_2S	Shah et al. (2015)
10	Silicalite-1	Alkanes	The AUA-4 force field can improve the prediction of the simulating alkanes adsorption. To predict the heat of the adsorption with a high level of accuracy	Pascual et al. (2003)

Table 3 (continued)

No.	Zeolite type	Adsorption/diffusion element	Main findings	Refs
11	ZIF-95, ZIF-100	H_2, N_2, methane	The capacity of ZIF-100 for the adsorption of smaller molecules is higher than ZIF-95, while ZIF-95 is more efficient for the adsorption of larger molecules. Due to higher interactions between gas molecules, the adsorption in both zeolites is higher in cryogenic temperature	Prakash et al. (2013)
12	NaY	*p*-xylene/*m*-xylene	The zeolite has a higher affinity toward *m*-xylene. The simulation could predict the adsorption process accurately. Both xylene isomers are situated in super cages of the zeolite after adsorption	Lachet et al. (1998)
13	Faujasite	*p*-xylene/*m*-xylene	The larger the extra-framework cation is, the lower the capacity of the adsorption is. The size of the cation does not have any effect on the adsorption selectivity. Y faujasites containing small monovalent cations have a higher affinity toward *m*-xylene	Lachet et al. (2001)
14	ACO, MEP, ASV, ANA, RWY, and RH	H_2	As the temperature increases, the adsorption capacity of the zeolites decreases. An increment of the pressure increases the hydrogen uptake of the zeolites. Moreover, zeolites with high pore diameter have a high tendency for hydrogen adsorption	Rahmati and Modarress (2009b)
15	IHW, IWV, SIV, UFI, and MS	N_2	At high pressures, the adsorption of nitrogen does not depend on the temperature significantly. In high pressures, the dependence between nitrogen uptake and pressure is nearly linear. Zeolites with higher pore volume have a higher capability for nitrogen uptake	Rahmati and Modarress (2009a)
16	Na-ZSM-5	CO_2, N_2	The higher amount of cations in the zeolite leads to an increment of the capacity of the adsorption. The molecules are mostly located in zigzag and straight channels	Newsome et al. (2014)
17	ZIF-8, ZIF-8-NH2, and ZIF-8-(NH2)2. ZIF-8	CO_2	The capacity of ZIF-8 for CO_2 capture can be enhanced using a modification of the zeolite with amine groups	Liu et al. 2013)
18	RuX, PdX	H_2	At 77 k, the increment in the exchanged cations' content leads to the hydrogen uptake decrement. At 303 K and 5 bar, the adsorption of hydrogen reaches a maximum amount for PdX zeolite. Owing to the chemical interaction between hydrogen and the exchanged cations, chemisorption of hydrogen happens at 303 K and 330 K	Prasanth et al. (2008)

Table 3 (continued)

No.	Zeolite type	Adsorption/diffusion element	Main findings	Refs
20	NaA, NaX	CO_2	The capacity of NaX for the CO_2 adsorption is higher than NaA. The heat of the adsorption for NaA is high. The higher the pressure is, the more carbon dioxide is adsorbed into both zeolites, shown schematically in Fig. 9	Liu and Yang (2006)
21	CHA, AFX, and ERI	n-alkanes	In lower pressures, the adsorption capacity of the heavier n-alkanes is higher, while in higher pressures, a reversal in the adsorption in terms of the selectivity between longer and smaller n-alkanes is witnessed. The diffusion and location of n-alkanes within CHA is shown schematically in Fig. 10	Krishna and Baten (2008)
22	ZIF-8, ZIF-90	Ethanol, methanol	The affinity of the zeolites is a little higher for ethanol than for methanol. Owing to the hydrogen bonding contained by ZIF-90, the capacity of this zeolite for the adsorption of the alcohol is higher than methanol	Gee et al. (2013)
23	FAU	CO_2, CH_4	NaX has a higher affinity toward CO_2 and CH_4 than NaY. The arrangement of the adsorbed molecules is more ordered in NaX	Zhang et al. (2014)

Furthermore, the capacity of adsorbents can be anticipated using molecular simulation techniques with an acceptable accuracy level. According to the enhanced development of the capability of the computer systems, it is expected that molecular simulation techniques will achieve a unique position for investigating the chemical process, including adsorption processes. For instance, there is a need to implement simulation when different sorts of pollutants are expected to be adsorbed on zeolites, like dyes, heavy metal ions, proteins found in biomedical wastewater, CO_x, SO_x, and NO_x. To date, some challenging aspects of molecular simulation of adsorption of pollutants by the zeolitic structures, to name: (1) the lack of experimental data on newly developed or sometimes theoretically born structures to validate models; (2) the number of hypotheses in simulations, mainly arising from the complexity of structures; (3) the size and distribution of pores and involvement of the porosity in simulations, which make computations timely and sometimes impossible; (4) the need for finding model parameters (coefficients of model and potential functions); and (5) more particularly, the inability of explaining the underlying mechanisms behind adsorption of pollutants by complex and hybrid zeolitic structures.

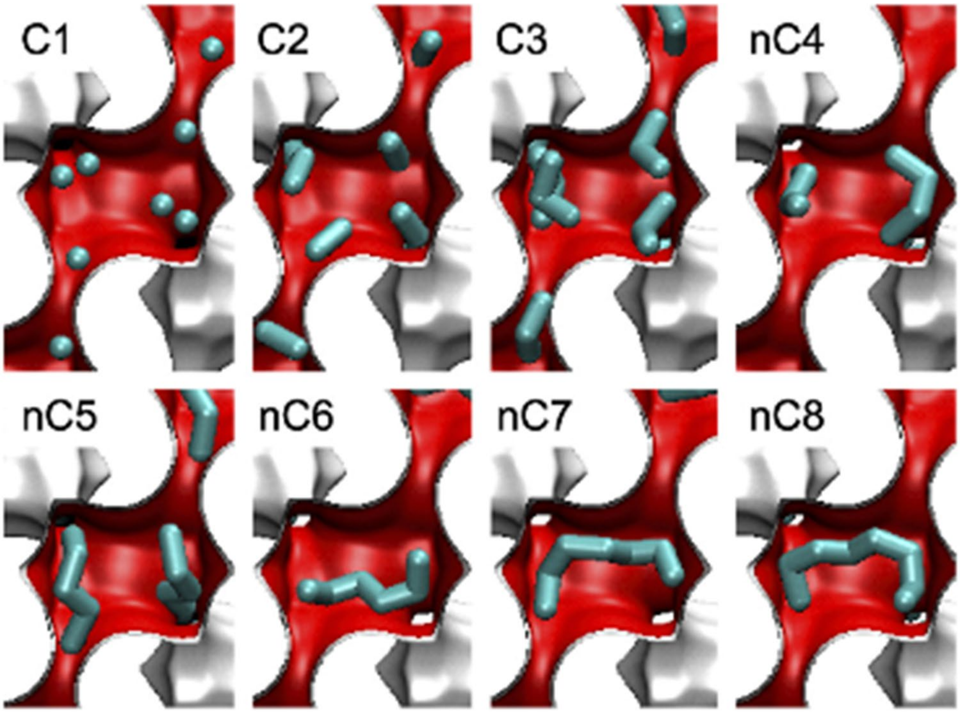


Fig. 11 Location of *n*-alkanes in the cages of CHA type zeolite (Krishna and Baten 2008)

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Declarations

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