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Grand canonical Monte Carlo simulation of isotherm for hydrogen adsorption on nanoporous siliceous zeolites at room temperature

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ABSTRACT

Zeolites belong to a most prominent class of nanoporous materials which have been considered as potential sorbents for hydrogen storage. The adsorption of hydrogen molecules on purely siliceous zeolites such as ACO, MEP, ASV, ANA, RWY, and RHO, which encompass a range of different pore structures and their chemical compositions has been simulated employing Grand Canonical Monte Carlo (GCMC) procedure for a temperature range of 250–325 K, and a pressure range of 0–10 kbar. The effects of pore structure of zeolites, temperature and pressure on the hydrogen adsorption has been examined. The results clearly show that the number of adsorbed hydrogen molecules at high pressure, only depends on pore diameter, and the temperature effect on the adsorption decreases with decrease in the number of adsorbed of hydrogen molecules.

1. Introduction

Hydrogen and fuel cells open the way to integrated "open energy systems" that simultaneously address all of the major energy and environmental challenges, and have the flexibility to adapt to the diverse and intermittent renewable energy sources that will be available in the world [1–5]. Thus, the use of hydrogen could drastically reduce greenhouse gas emissions from the energy sector. Fuel cells are intrinsically clean and very efficient and capable of converting hydrogen and other fuels to electricity, heat and power [6–9].

Low-cost production of hydrogen from water and its utilization on a massive scale as an energy carrier, substituting for fossil fuels, would constitute a major advance toward alleviation of the build up of atmospheric carbon dioxide and its associated potential effect on global climate change [3,10,11]. Hydrogen can be substituted for carbon-based fuel for transportation, for electric power generation using fuel cells, and for process heat [11–14]. For transportation applications, hydrogen can be used to drive a fuel cell power train or can be used directly in an internal combustion engine; the former eliminates all undesirable emissions [14,15]. However, there are many significant challenges for implementing all the components of a complete energy system based on hydrogen [1,16,17]. Despite these challenges, there is a global interest in hydrogen as an energy carrier with commercial competition emerging for the government. The transition to a full hydrogen system will be lengthy, costly and will require significant research and development.

The challenge is especially demanding for on-board storage in road vehicles. A number of novel storage techniques are being investigated to complement the currently available methods where hydrogen is stored in gaseous (adsorption) [8]. The methods of storage currently under consideration include high pressure gas, liquid hydrogen, adsorption on porous materials, complex hydrides and hydrogen intercalation in metals [2,9,12,13,16]. None of these methods completely satisfy all the criteria for the amount of hydrogen that can be supplied from a given weight or volume of tank for transport purposes.

Hydrogen storage is a key enabling technology for the extensive use of hydrogen as an energy carrier. Therefore, the aim is to develop economically and environmentally attractive solutions for storage options. These systems will be producible at industrial scale and will meet commercially viable goals for cost, energy density and durability. In addition, achieving sufficient hydrogen storage capacity for adequate vehicle range is a major technology goal.

The US Department of Energy has stated that storage materials need to have a storage capacity more than 6% of their own body weight to be practical for transportation uses [18]. Several experiments in carbon nanotubes [17,19–22] and metal organic frameworks [23–28] showed somedeal low storage performance from 0.2 up to 1% and 0.2 up to 1.6% of their own weight in hydrogen at room temperature, respectively. Recent investigations

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are still in progress to understand the real potential of such materials for hydrogen storage. The focus is on improved, low-cost and high storage manufacturing techniques.

Zeolites are hydrated aluminosilicate minerals and have a nanoporous structure [29,30]. They are widely used as ion-exchange beds in domestic and commercial water purification, softening, and other applications. In chemical processes, zeolites are used to separate molecules and gases (only molecules of certain sizes and shapes can pass through), as traps for molecules so they can be analyzed. However, at present, the true potential to improved the hydrogen storage [29,31–38]. They are of interest because of their high thermal stability, low-cost, high bulk density, and adjustable composition [1,3].

It has been reported that the amount of material adsorbed on a zeolite depends on the framework structure and chemical composition of that zeolite. The shape of the channels and the high surface area as well as the interaction between the zeolite framework and hydrogen are determinant factors to control these properties [10].

However, in this paper, we report physisorption of hydrogen molecules on purely siliceous zeolites such as MEP, ACO, ANA, ASV, RWY, and RHO has been simulated employing GCMC procedure. Moreover, the effects of zeolite pore structure, temperatures and

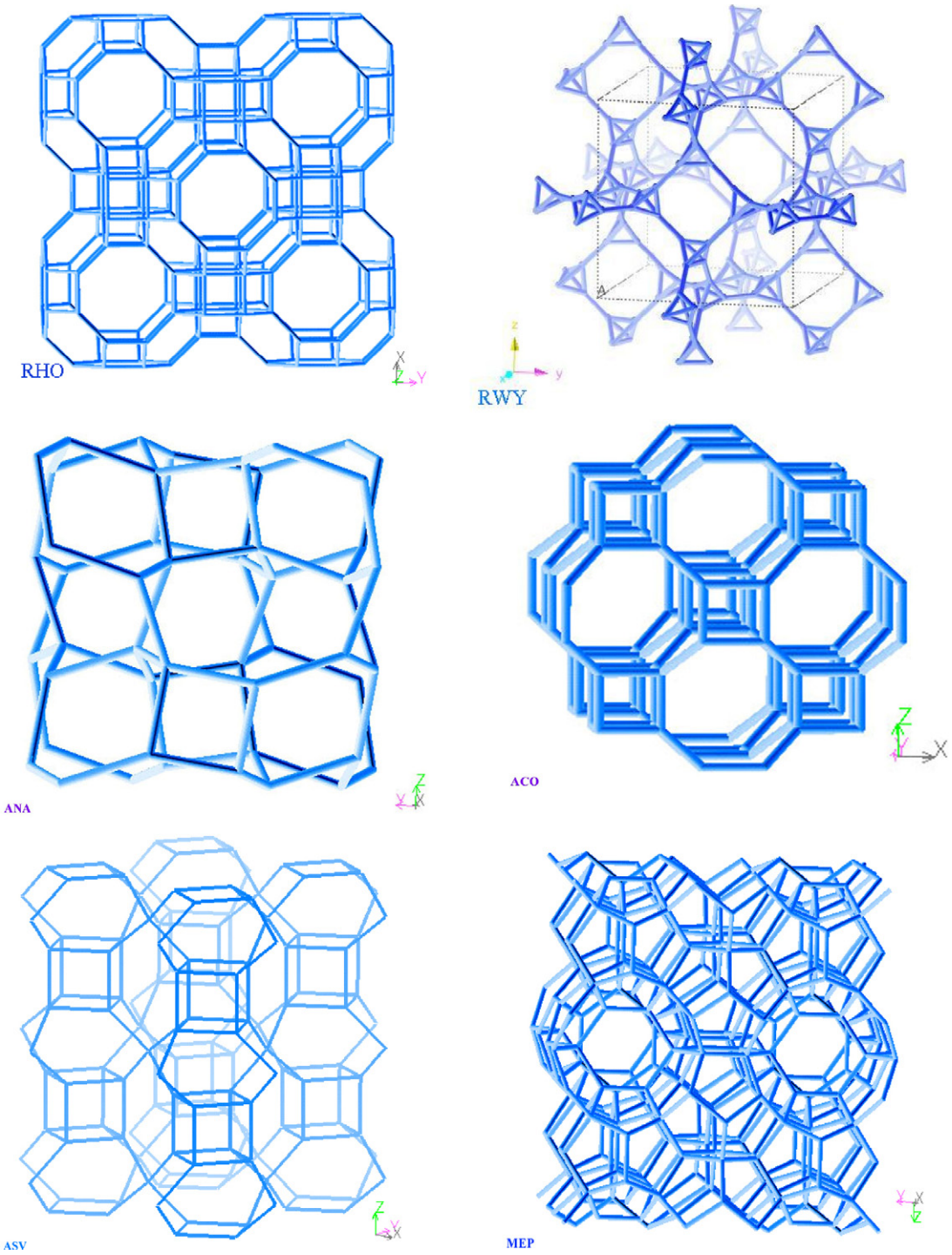

Fig. 1. Framework structures of zeolite such as ACO, MEP, ASV, ANA, RWY and RHO.