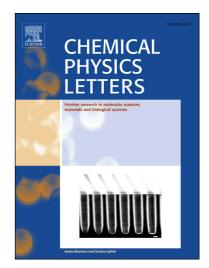# Accepted Manuscript

Research paper

Path integral centroid molecular dynamics simulation of para-hydrogen sandwiched by graphene sheets

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Abstract

The carbon-hydrogen composite systems of para-hydrogen (p-H_2) sandwiched by a couple of graphene sheets have been investigated by means of path integral centroid molecular dynamics simulations at 17 K. It has been shown that sandwiched hydrogen is liquid-like but p-H_2 molecules are preferably adsorbed onto the graphene sheets because of attractive graphene-hydrogen interaction. The diffusion coefficient of p-H_2 molecules in the direction parallel to the graphene sheets is comparable to that in pure liquid p-H_2. There exists a characteristic mode of 140 cm^{-1} of the p-H_2 molecules, attributed to adsorption-binding motion perpendicular to the graphene sheets.

1. Introduction

In recent decades the adsorption of hydrogen in carbon materials such as nanotubes, nanohorns, and graphite has attracted much attention in the prospect of possible capability of energy source, and has extensively been investigated by means of computational simulations [1-19]. Prior to such computational works on the carbon-hydrogen composite materials, in 1973 Steele et al. studied the physical interaction of gases with solids to give the potentials for physisorption [20]. Using Steele's potential between hydrogen and graphite basal plane, Darkrim et al. investigated the adsorption of hydrogen molecules on graphite surfaces at 293 and 77 K by means of grand canonical Monte Carlo (MC) simulation to provide adsorption isotherms and hydrogen density distributions [17].

On the other hand, it is general that hydrogen molecules in condensed phases exhibit quantum effects, as are manifested as the thermal de Broglie wavelength which is comparable to intermolecular distances at low temperatures. In order to simulate hydrogen systems, it is therefore needed to include such quantum nature in the framework of

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