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Theoretical Simulations of Fundamental Processes of the H_2 Formation Reaction on Dust Surfaces

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Abstract. Classical molecular dynamics (MD) computer simulations were performed to investigate the whole fundamental processes of the H_2 formation reaction on the amorphous water ice as a model surface of icy mantles of dust grains. The product energy distribution and formation pumping mechanism of H_2 formed on dust grains were also examined.

1. Introduction

Since the homonuclear diatomic radiative association cannot occur efficiently and three-body reactions are excluded in gas phase in interstellar space, molecular hydrogen ought to be formed on the surface of cosmic dust grains. Fundamental processes of H_2 formation on dust surfaces are considered as follows: 1) sticking process of incident H atoms onto the dust surface, 2) diffusion process of H atoms on the dust surface, 3) reaction process of two H atoms on the dust surface, and 4) ejection process of the product H_2 molecule from the dust surface back into gas phase (see Fig. 1).

There have been many theoretical studies relating to the H_2 formation process on dust grains (see references in Takahashi 2000). Recently, there have been also several experimental studies to reproduce the H_2 formation process on cosmic dust grain analogues (see references in Takahashi 2000). However, there have been no theoretical studies which treated all fundamental processes by a single model, and it should be difficult to resolute pure fundamental processes experimentally. On the contrary, in the present theoretical studies by us (see, e.g., Takahashi, Masuda & Nagaoka 1999a,b; Takahashi & Williams 2000), all fundamental processes of H_2 formation on the surface of dust grains were examined throughout by a single realistic model, based on classical molecular dynamics (MD) computer simulations.

2. MD Simulation of H_2 Formation on Icy Mantles

The MD simulation is a well established technique for studying molecular processes in the field of physical chemistry. In this simulation, Newtonian equations of motions are solved numerically to obtain positions, velocities, and forces as functions of time for particles interacting with each other.

For the first stage of the present MD simulation, as a realistic model surface of icy mantles of dust grains, the slab-shaped amorphous water ice was generated

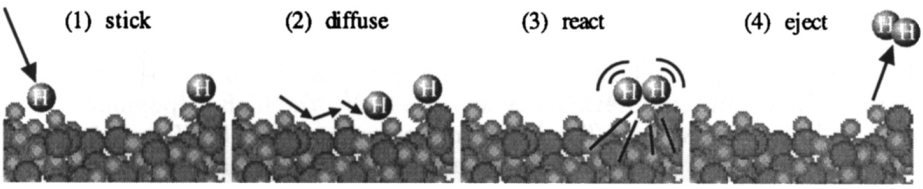

Figure 1. Fundamental processes of H_2 formation on dust surfaces.

at 10 K and 70 K under periodic boundary conditions. The volume of the slab in the unit cell was about 40 Å × 40 Å × 20 Å and 1000 H_2O molecules were contained in it. For the second stage, two H atoms with kinetic temperatures of 10–350 K were thrown one after one onto the amorphous water ice slab to reproduce the H_2 formation reaction on the surface of icy mantles. Here, a pair of H atoms with antiparallel electronic spins were simply assumed. The total potential of the present system was given as the sum of pair potentials for H_2O–H_2O, H_2O–H, and H–H. As for the intramolecular potential of H_2O, a spring-type potential was also taken into account.

3. Fundamental Processes of H_2 Formation on Dust Surfaces

The summary of the results of MD simulation about the four fundamental processes of H_2 formation on icy mantles is described in the following.

(1) For the sticking process, it was found that the sticking probability of the incident H atom onto the icy surface is almost unity at less than 70 K and that it decreases with increasing kinetic temperatures of the incident H atom.

(2) For the diffusion process, it was found that the incident H atom initially diffuses on the dust surface via thermal hopping mechanism for just a short time after sticking and then it becomes always trapped in one of stable sites on the amorphous water ice. The migration length and time were obtained for the mobility of the incident H atom before trapping, and timescales of thermal diffusion and desorption of the trapped H atom were estimated for the mobility after trapping.

(3) For the reaction process, the following three reaction patterns were observed: a) H_2 was produced via the Langmuir-Hinshelwood mechanism, b) H_2 was produced via the Eley-Rideal mechanism, and c) almost elastic collision of two H atoms occurred without H_2 being formed. It was found that two H atoms began to react when they encountered at the distance less than 3.5 Å, where the H–H interaction overcomes the H–surface interaction. The production probability, defined as the probability that H_2 is produced after two H atoms (with antiparallel electronic spins) encountered on the dust surface was found to be near unity.

(4) For the ejection process, it was found that the product H_2 was always subsequently ejected after the reaction process via the direct ejection mechanism, in that, a part of the H_2 formation energy was used for the product H_2 itself to escape from the dust surface. The average ejection time scale was found to be about 0.5 ps (picoseconds, 1 ps = 10^{-12} s).

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4. Formation Pumping Mechanism

The product energy analysis of H_2 ejected from the icy surface was also performed. The resulting vibrational energy level with the highest population was found to be around v = 8. The H_2 formation energy (= 4.5 eV) was found to be distributed to the vibrational, rotational, and translational energies of H_2 by about 74 %, 12 %, and 10 %, respectively. The energy absorbed by the ice was found to be only about 4 %.

The formation pumping mechanism can be explained as follows. The H_2 formation energy or H–H bond energy originally resides in the vibrational energy of the product H_2. Through the H–surface interaction, the H_2 formation energy should be absorbed by the dust and partially converted to the rotational and translational energies of H_2. If the H–surface interaction and the ejection time scale of H_2 is limited, energy conversion cannot be completed, and the product H_2 is still vibrationally excited.

The formation pumping levels of H_2 on various dust surfaces are exhibited in Table 1, where the results about silicate and carbonaceous dust surfaces are taken from Duley & Williams (1986) and Farebrother et al. (2000), respectively. It is found that as large as the H–surface interaction is, more energy is absorbed by the dust and less internal energy is left in the product H_2. However, H_2 can be still vibrationally excited on each dust surface.

In conclusion, I would like to contend that interstellar H_2 newly formed on dust grains should be vibrationally excited by the formation pumping mechanism. As was suggested by Duley and Williams (1993), it tells us that the rovibrational emission spectrum of H_2 might be detectable in regions without a source of UV pumping or dynamical excitation.

Table 1. Formation pumping levels of H_2 on various dust surfaces.

Dust surface	icy mantles	silicate dust	carbonaceous dust
H–surface interaction	weak	middle	strong
	< 0.1 eV	~ 0.4 eV	~ 1.6 eV
Main vibrational level	v = 8	$v \leq 7$	v = 2

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