Formation of H_2 in the Interstellar Medium at High Temperature

Wasim Iqbal[1], Kinsuk Acharyya[1] and Eric Herbst[2]

1. S. N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata 700098, India,

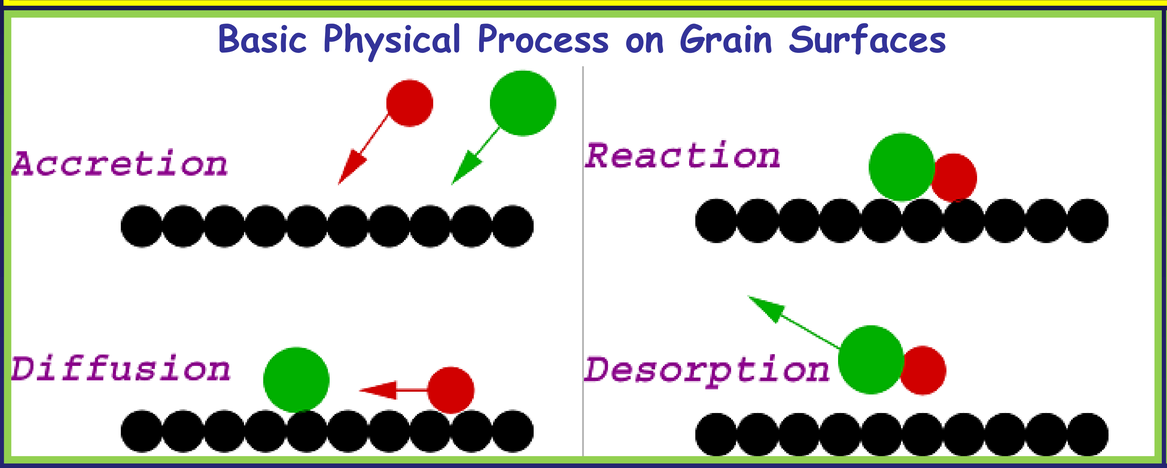
2. Department of Chemistry, University of Virginia, USA

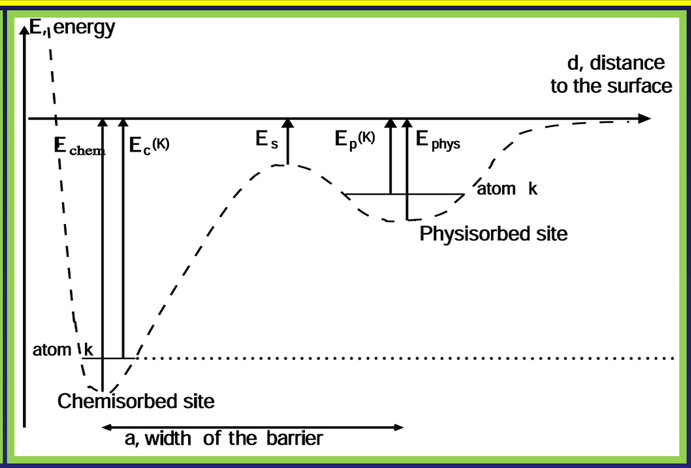
CENTRE FOR BASIC SCIENCES 1986 — S. N. BOSE NATIONAL — 1894-1974 — विज्ञानेन परिपश्यन्ति धीराः

Abstract: We used the continuous-time random-walk (CTRW) Monte Carlo technique to study the formation of H_2 on the surface of interstellar dust grains with both physisorption and chemisorption sites on olivine and carbonaceous material. We have considered hydrogen atom mobility due to both thermal hopping and quantum mechanical tunneling. In addition, we have also considered rough surfaces with multiple binding sites. Tunneling is found to dominate the surface chemistry at low temperature, but as the temperature increases, the scenario changes. The inclusion of chemisorption sites can provide a meaningful efficiency for H_2 production up to as high a temperature as 700 K depending upon the depth of the chemisorption well. We found that over virtually the entire temperature range studied, the use of rate equations overestimates the H_2 formation rate. This overestimate is large at high temperatures, due to very low surface residence times.

Introduction: H_2 is the simplest and most abundant molecule in the interstellar medium. Almost all of the elemental hydrogen in translucent and dense molecular clouds is in its molecular form, which is also the most abundant molecular species in diffuse clouds. Moreover, H_2 is observed in large quantities in various galactic and extragalactic sources such as photon dominated regions (PDRs), jets, shocks, outflows of planetary nebula, active galactic nuclei (AGNs), and supernova remnants. In spite of its overwhelming presence, the process of H_2 formation in these diverse environments is not entirely clear. Since H_2 plays a crucial role in the dynamical and chemical evolution of the interstellar medium (ISM), the study of how H_2 is formed remains of fundamental importance.

Model: In the kinetic Monte Carlo technique, atoms and molecules are treated individually and their surface motions (accretion, hopping/tunneling, desorption, recombination) take place on a lattice depending upon the values of random numbers called in a continuous time frame. In order to mimic the spherical grain structure, we assumed periodic boundary conditions; i.e., a species that leaves the lattice on one side enters back from the opposite side. We considered three different models for both olivine and carbonaceous grain, which differ in physisorption and chemisorption energies and barrier width between them (as shown in Table 1).





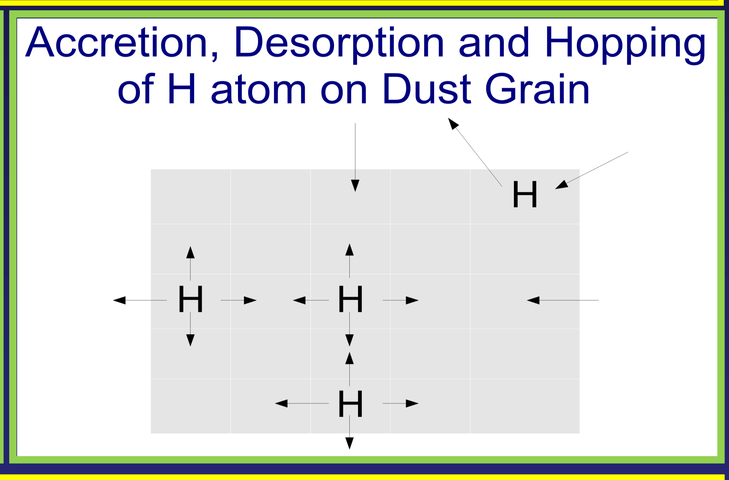
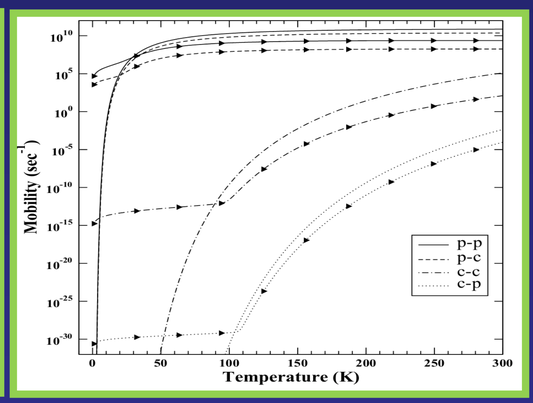


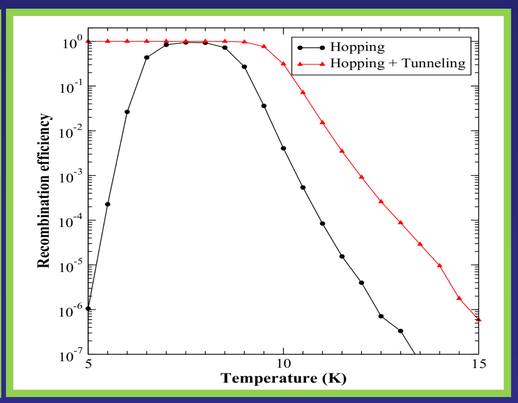
Table 1: Potential Height and Width Parameters

Surface	a Å	A Å	E_{phys} K	E_{chem} K	E_s K	E_{sp} K	E_{sc} K	E_{H_2} K	μ	Model
Olivine	2.5	2	400	10000	100	100	5000	300	0	O1
Carbon	2.5	2	780	14000	100	100	7000	300	0	C1
Olivine	2.5	2	400	30000	100	100	15000	300	0	O2
Carbon	2.5	2	780	30000	100	100	15000	300	0	C2
Olivine	3	2	660	30000	100	100	15000	300	0	O3
Carbon	3	2	860	30000	330	100	15000	300	0	C3

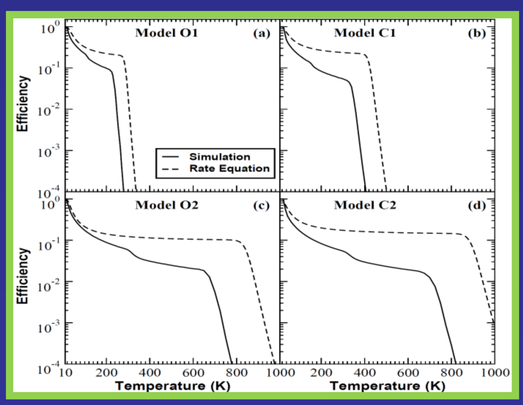
Binding energies of H atom on the surface of the dust grain, used in the different models.



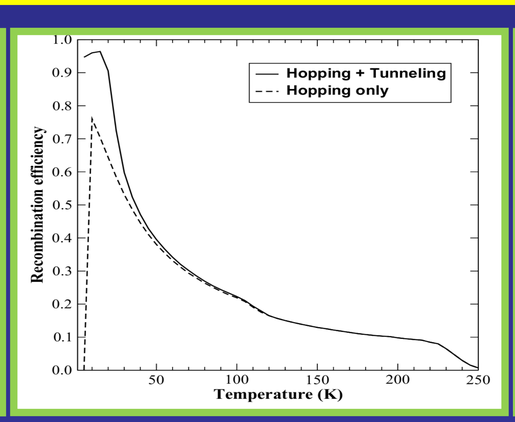
Mobility of H atoms between different types of binding site on the dust surface for O1 model.



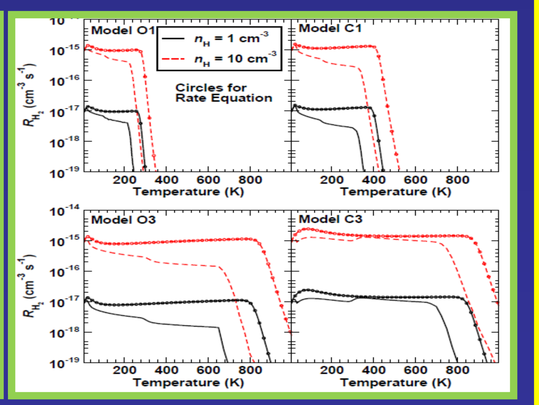
Efficiency as function of temperature of dust grain for O1 model excluding chemisorption sites.



Efficiency as a function of temperature for O1 & O2 models including chemisorption sites.



Effect of tunneling on efficiency of H_2 formatiom for O1 model.



Rate of H_2 formation as a function of temperature for different models.

Summary

1. Reasonable efficiencies for H_2 recombination can occur at temperatures up to 700 K if deep chemisorption wells (30,000 K) coexist with weak physisorption sites.

2. MC results significantly differ from the rate equation approach. The later approach overestimates the efficiency of H_2 production at virtually all temperatures studied, especially high temperatures, and gives a much wider range of temperatures for reasonable production of H_2, approaching a high-temperature limit of 1000 K for models with deep chemisorption wells.

3. Both the Monte Carlo method and the rate equation method show that the temperature range of efficient recombination decreases as the chemisorption wells are made more shallow, and that for pure physisorption the temperature range is miniscule and at very low temperature only for both olivine and carbon, confirming the work of Katz et al. (1999).

4. Using a rough rather than a flat surface enlarges the temperature range somewhat, as in the prior work of Cuppen & Herbst (2007), but the effect of roughness is much smaller than the effect of even relatively weak chemisorption wells.

5. We investigated the mechanism of H_2 formation in some detail, and confirmed the result of Cazaux & Tielens (2004) that tunneling, if it actually occurs, plays a significant role in H_2 formation at low temperatures, but with the increase of surface temperature, the thermal mobility of adatoms increases rapidly and thermal hopping of H atoms dominates.

6. We also investigated the dependence of the recombination efficiency over a wide temperature range on the hydrogen atom flux and on grain size. For grains with physisorption and chemisorption sites, we found that the effects were strong only at the highest temperatures, where higher fluxes and larger grain sizes lead to higher efficiencies over larger temperature ranges.

Refrences: **1.** Cazaux, S., & Spaans, M., 2004, Apj, 611, 40, **2.** Cazaux, S., & Tielens, A. G. G. M., 2002, ApJ, 575, L29, **3.** Cazaux, S., & Tielens, A. G..G.M., 2004, ApJ, 604, 222, **4.** Chang, Q., Cuppen, H.M., & Herbst, E., 2005, A&A, 434, 599, **5.** Chang, Q., Cuppen, H.M., & Herbst, E., 2006, A&A, 458, 497, **6.** Cuppen, H. M., & Herbst, E. 2007, ApJ, 668, 294. **7.** Katz N., Furman I., Biham O., Pirronello V., & Vidali G., 1999, ApJ., 522, 305, **8.** Iqbal W., Acharyya K., & Herbst E. (submitted ApJ).