

The formation of H₂ and HD with the master equation approach

Ofer Biham, Azi Lipshtat and Hagai B. Perets

¹Racah Institute of Physics, The Hebrew University, Jerusalem, 91904, Israel ²Department of Physics, Weizmann Institute of Science, Rehovot 76100, Israel

Abstract.

While most chemical reactions in the interstellar medium take place in the gas phase, those occurring on the surfaces of dust grains are of fundamental importance. In particular, the formation of molecular hydrogen, which is the most abundant molecule in the Universe, takes place on dust grains. Molecular hydrogen plays a crucial role in the cooling processes that enable gravitational collapse and star formation. It is also a necessary component in the reaction networks that give rise to the chemical complexity observed in interstellar clouds.

In this talk I will show our analysis and interpretation of laboratory experiments by Vidali, Pirronello and collaborators, on molecular hydrogen formation on astrophysically relevant surfaces such as olivine, amorphous carbon (Katz et al. 1999) and amorphous ice (Perets et al. 2005, see also Hornekaer et al. 2003). The analysis is based on rate equations that are appropriate for macroscopic surfaces such as those used experimentally. The implications to the interstellar medium will then be considered. The results indicate that hydrogen recombination is efficient only within a narrow temperature range between 10 and 20 K. Observations show that molecular hydrogen is abundant also in warmer environments such as photon-dominated regions, where grain temperatures may reach 45 K. Possible explanations of this apparent discrepancy will be discussed, particularly the role of chemisorption sites (Cazaux & Tielens 2004) porosity and temperature fluctuations.

Due to the microscopic size of the dust grains in the interstellar medium, the mean-field approximation on which the rate equations are based may not apply. Stochastic calculations are needed, which take into account the discrete nature of the population of adsorbed atoms and molecules on the grain and their fluctuations. I will present such approach based on the master equation (Biham et al. 2001, Green et al. 2001). Using this methodology I will present results for the rate constant of molecular hydrogen formation, taking into account the size distribution of grains. The generalization to deuteration processes (Lipshtat et al. 2004) as well as to complex reaction networks of multiple species (Lipshtat & Biham 2004) on grain surfaces will also be discussed.

References

- Katz, N., Furman, I., Biham, O., Pirronello, V. & Vidali, G. 1999, *Astrophys. J.* 522, 305
Perets, H.B., Biham, O., Manicó, G., Pirronello, V., Roser, J., Swords, S. & Vidali, G. 2005 *Astrophys. J.*, 627, 850
Cazaux, S. & Tielens, A.G.G.M. 2004, *Astrophys. J.* 604, 222
Hornekaer, L., Baurichter, A., Petrunin, V. V., Field, D. & Luntz, A. C. 2003, *Science*, 302, 1943
Biham, O., Furman, I., Pirronello, V. & Vidali, G. 2001, *Astrophys. J.*, 553, 595
Green, N.J.B., Toniazzo, T., Pilling, M.J., Ruffle, D.P., Bell, N. & Hartquist, T.W. 2001 *Astron. Astrophys.* 375, 1111
Lipshtat, A., Biham, O. & Herbst, E. 2004 *Mon. Not. R. Astron. Soc.* 348, 1055
Lipshtat, A. & Biham, O. 2004 *Phys. Rev. Lett* 93, 170601