Dust temperature fluctuations and surface chemistry : H_2 formation

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Among dust grains, very small grains and PAHs are known to be of dominating importance for various physical processes, such as the photoelectric heating of the gas. The dust size distribution in the interstellar medium is believed to be so that despite big grains making up most of the dust mass, the smallest grains dominate the total available dust surface. Small grains are thus also the principal substrate for surface reactions, the most important of which is the formation of H_2.

Due to the small heat capacity of small grains, individual UV photons cause large spikes of their temperature. Such fluctuations have been studied in details for the purpose of modeling dust emission in the NIR. Yet surface chemistry models almost always assume a non-fluctuating grain temperature. While this assumption is reasonable for the complex surface chemistry occurring in dark cloud cores, it is much less justified for the formation of H_2 in UV-rich environments such as diffuse gas or bright PDRs.

Various mechanisms can contribute to H_2 formation. The Langmuir-Hinshelwood mechanism involves physisorbed atoms migrating on the surface, and was experimentally found to have a limited temperature range of efficiency (typically 10-20K), while ISO and Spitzer observations of PDRs found efficient formation despite warmer dust. Other mechanisms were proposed such as the Eley-Rideal mechanism, involving direct reaction between a chemisorbed atom and a gas atom, and insensitive to grain temperature.

We present here the first complete analytical treatment of the statistical problem of surface chemistry with fluctuating temperatures, using a master equation approach to follow exactly both the temperature and the population of adsorbed atoms. We apply this treatment to the Langmuir-Hinshelwood mechanism and find it to be much more efficient than expected in unshielded environments under moderate UV fields, as the grain average temperature is actually not representative of the cold state in which the grain spends most of its time between the short spikes. Another mechanism is still necessary to account for formation under strong UV fields, and the Eley-Rideal mechanism is found to retain most of its efficiency when temperature fluctuations are taken into account. Fast approximations of the exact results are also constructed. This method could be generalized to other surface reactions.

The effects of this new formalism on full cloud simulations are explored using the Meudon PDR code. Effects are found in tracers of the cloud edge (H_2, CH^+) but remain limited as the improved Langmuir-Hinshelwood formation is partly masked by the already efficient Eley-Rideal formation. The increase in Langmuir-Hinshelwood efficiency nevertheless allows more flexibility in the choice of the poorly known microphysical parameters of the Eley-Rideal mechanism, as will be demonstrated using the constraints of the observations of a few well known PDRs.