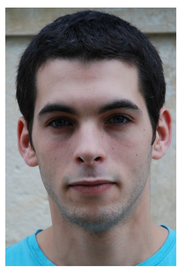
Energy dissipation on interstellar dust particles



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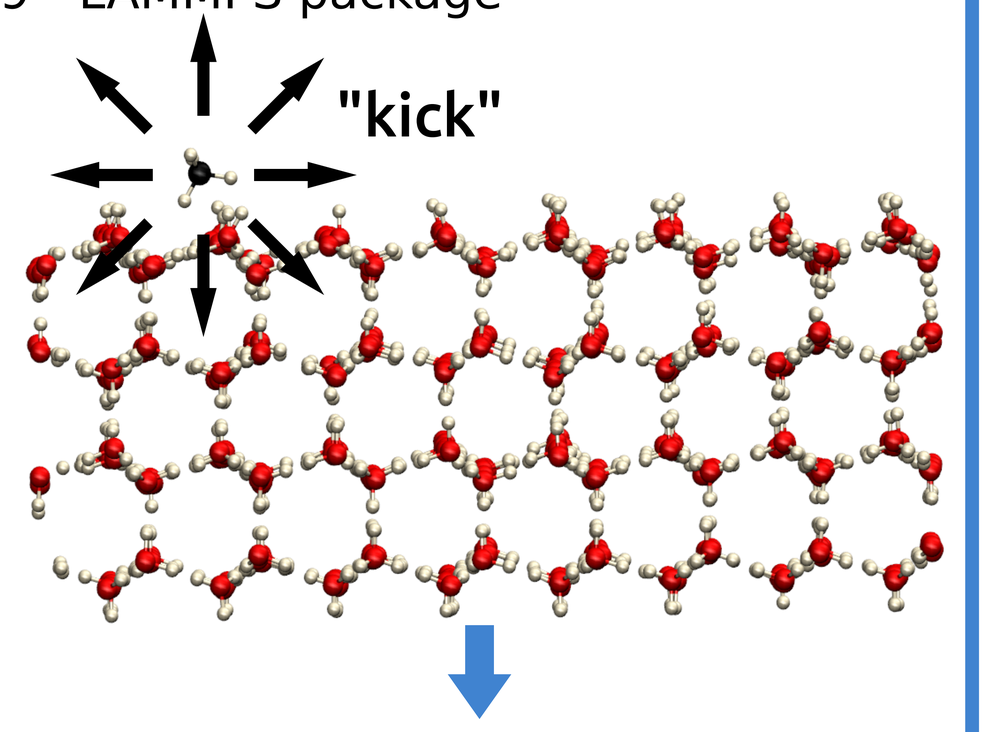
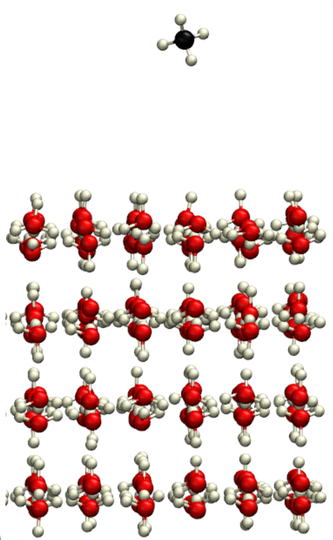
Context

Dust particles covered by icy mantles play a crucial catalytic role in the formation of molecules in the Interstellar Medium (ISM).This study consists in understanding the behaviour of three chemical compounds (CO_2, H_2O, CH_4) on icy grain surfaces to study the effect of mass, internal degrees of freedom and interactions with the surface.

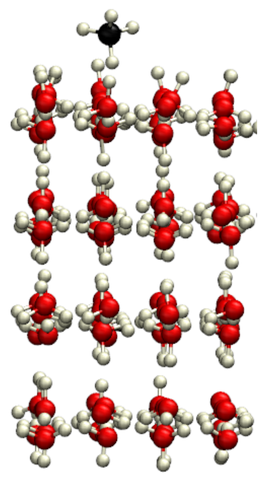
Methods

1 - 36400 MD simulations per species
2 - H disordered crystalline ice
3 - Random kick uniformally distributed in all directions
4 - E_{kick} = 1 - 4 eV
5 - 70 starting points
6 - NVE ensemble
7 - T = 10 K
8 - Δt = 0.2 fs, t_{max} = 20 ps
9 - LAMMPS package

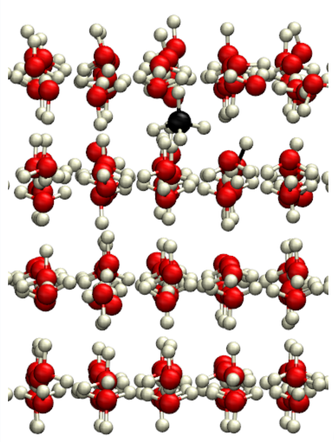




Desorption



Adsorption



Penetration

Conclusions

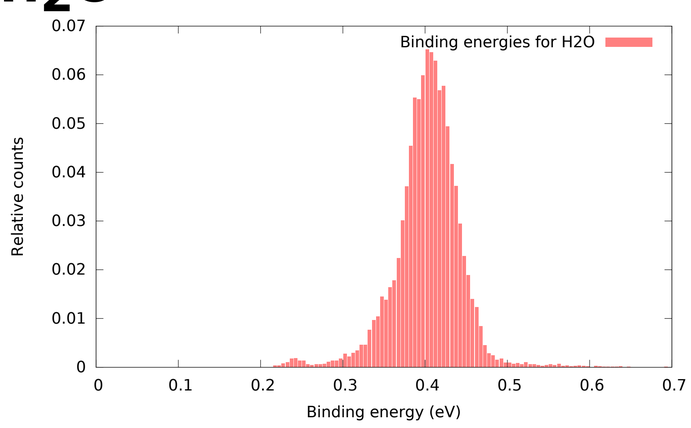
- The binding energy dictates the surface mobility and the desorption probability.
- Non-thermal diffusion increases the mobility of admolecules and increases the probability of following reactions.

[1] L. J. Karssemeijer, G. A. de Wijs and H. M. Cuppen, *Phys. Chem. Chem. Phys.*, **2014**,16, 15630-15639

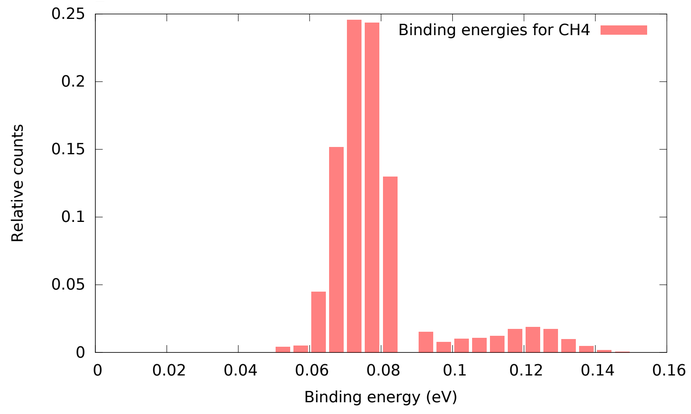
Results

Binding energies

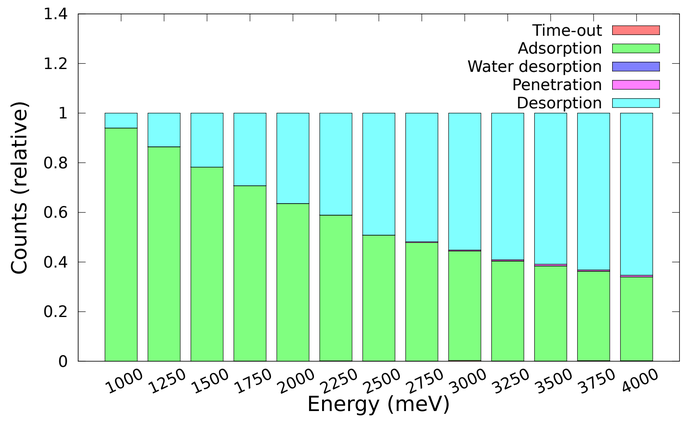
H_2O

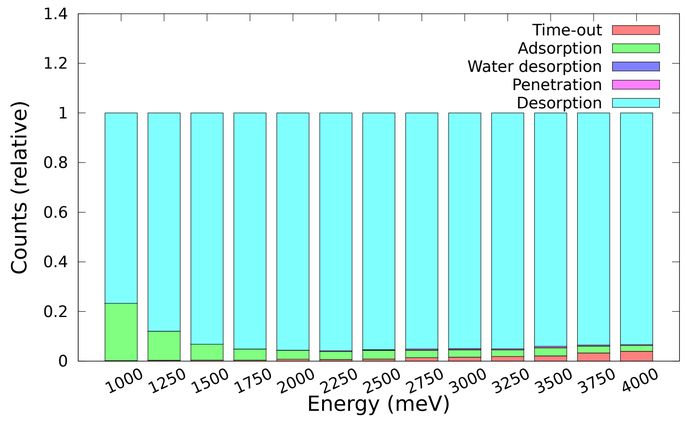


CH_4



Outcome statistics



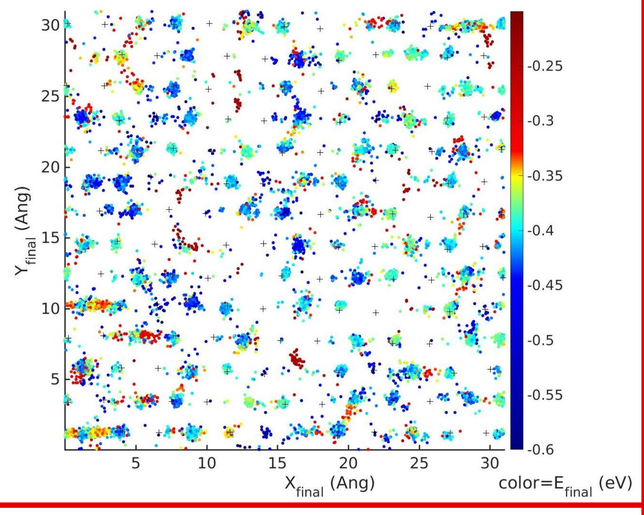


→ Desorption directly correlated with binding energy not with internal degrees of freedom or mass. For CO_2, we observe an intermediate behaviour in agreement with reference [1].

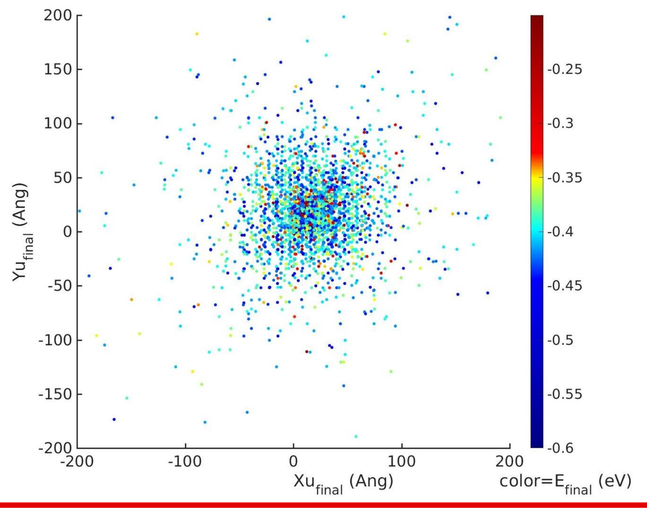
Travelled distance

Wrapped coordinates

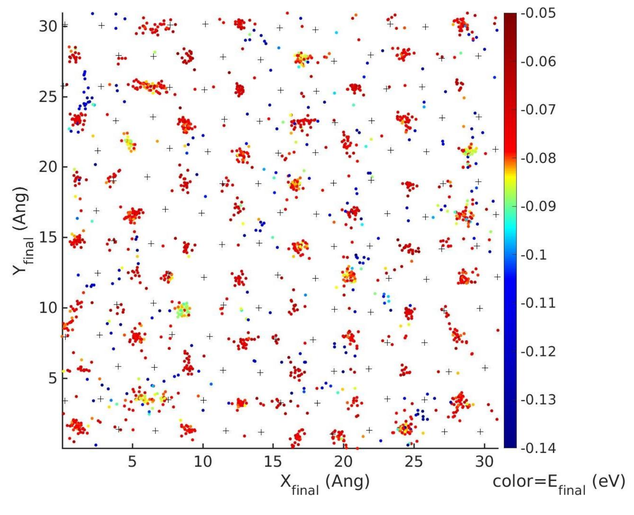
H_2O

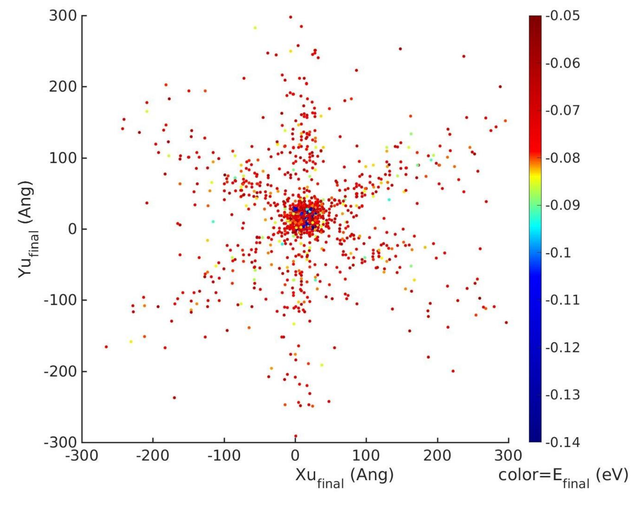


Unwrapped coordinates



CH_4





→ CH4 moves further than H_2O and the CH_4 pattern has an hexagonal shape. For CO_2, we observe an intermediate behaviour.