

HCO· formation at the interface with crystalline models of icy mantles: insights from MD simulations

<u>S. Pantaleone</u>, J. Enrique-Romero, A. Rimola, P. Ugliengo, C. Ceccarelli, N. Balucani, D. Skouteris





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Reactivities on ice surfaces: an atomistic view



Boogert et al. 2015

But what is actually happening?

Computational quantum chemistry is an extremely powerful tool to answer the question.

See also **posters** by **Fanny Vazart** & **Joan Enrique-Romero** downstairs

Static calculations: what can we simulate?



Elastic properties of skin/tendons

A little improvement: molecular dynamics





See also **posters** by **Fanny Vazart & Joan Enrique-Romero** downstairs

Ice surface modelling









Where does the released reaction energy go?

1. To the ice?

2. Will the molecule break?

3. Will the molecule desorb



How do we answer these questions? Molecular dynamics!

Pilot study: H + CO

Computational Details

- Package: CP2K
- Method: PBE (Density Functional Theory)
- Basis set:
 - Core electrons (GTH pseudopotential)
 - Valence electrons (GPW TZV2P)
- Dispersion correction: Grimme D3
- MD simulations:
 - Ice thermalization @ 10 K (NVT ensemble)
 - Production (NVE ensemble)
 - t-step: 1 fs

GTH = Goedecker-Teter-Hutter GPW = Gaussian plane waves: basis of Gaussian functions and auxiliary plabne waves





HCO· reaction profiles



-137.2

2.38

2.23



The reaction has a barrier so that in the ISM it occurs via tunnelling. Here we simulate how the energy is dispersed, therefore we start from the TS.

HCO· in gas phase: answer 2, the molecule breaks



H-C distance



Potential energy



HCO energy dissipation: answer 1, into the ice



 1- Energy is dissipated into the "bulk" in ps timescale
2- HCO remains stuck.



CONCLUSIONS

Where does the released reaction energy go?

1. To the ice?

2. Will the molecule break?









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CONCLUSIONS

Where does the released reaction energy go?





How do we answer these questions? Molecular dynamics!

CONCLUSIONS

Where does the released reaction energy go?





How do we answer these questions? Molecular dynamics!

Prospectives: H₂ on the ice surface





Acknowledgements





Stefano Ferrero

Piero Ugliengo



Lorenzo Zamirri





Nadia Balucani



Dimitrios Skouteris



Albert Rimola



UAB

Universitat Autònoma de Barcelona

Mariona Sodupe





Center







TS of 1.27 kJ/mol

