Machine Learning Meets Surface Astrochemistry

G. Molpeceres[1]

[1]*Institute for Theoretical Chemistry University of Stuttgart Pfaffenwaldring 55, 70569 Stuttgart, Germany*

Surface reactions play a vital role in the chemistry occurring on interstellar mediums (ISM). In particular, under the cold conditions of a molecular cloud (~10-20 K), adsorbates (atoms, radicals and molecules) accrete, diffuse, react and desorb on top of ice-covered dust grains [1]. The chemical composition of these ices is varied and depends on the cloud's evolutionary stage, e.g. water ice dominates the early stages [2]. At the same time, CO and CO_2 are prevalent in later stages. Moreover, interstellar ices are usually amorphous, presenting a wide range of binding sites for adsorbates to perform the aforementioned processes [2]. It appears evident that, given the complexity of the substrates, the dynamics of adsorbates on interstellar ices are essentially non-local, meaning that a particular process depends significantly on the binding site under consideration. This condition imposes a constraint on computational studies of interstellar surface chemistry, requiring extensive sampling and considerably increasing the computational cost for constructing reliable models. Several approaches are employed in the literature to reduce this cost, i.e. cluster models [3], periodic models, [4] QM/MM models [5] and recently, machine-learned models [6]. In this contribution, I will present our recent efforts in the application of neural-network potentials [7] to surface astrochemistry, putting the focus on the simulation of:

1. Adsorption and desorption (calculation of sticking coefficients and desorption rate constants) [6];
2. Diffusion (estimation of diffusion coefficients and hopping rate constants) [8];
3. Reaction (chemical desorption vs energy dissipation) [9].

References

[1] Cuppen, H.M. et al. *Space Sci. Rev.* **212,** 1-58 (2017).

[2] Boogert, A.C.A., Gerakines, P.A. & Whittet, D.C.B. *Annu. Rev. Astron. Astrophys.* **53**, 541–581 (2015).

[3] Shimonishi, T., Nakatani, N., Furuya, K. & Hama, T. *Astrophys. J.* **855**, 27 (2018), Bovolenta, G. et al. *Mol. Astrophys.* **21**, 100095 (2020).

[4] Ferrero, S. et al. *Astrophys. J.* **904**, 11 (2020).

[5] Molpeceres, G. & Kästner, J. *Phys. Chem. Chem. Phys.* **22**, 7552–7563 (2020), Sameera, W.M.C. et al. *J. Phys. Chem. A* **125**, 387–393 (2021), Duflot, D., Toubin, C. & Monnerville, M. *Front. Astron. Sp. Sci.* **8**, 24 (2021).

[6] Molpeceres, G., Zaverkin, V. & Kästner, J. *Mon. Not. R. Astron. Soc.* **499**, 1373–1384 (2020), Molpeceres, G., Zaverkin, V., Watanabe, N. & Kastner, J. *Astron. Astrophys.* **648**, A84 (2021).

[7] Zaverkin, V. & Kästner, J. *J. Chem. Theory Comput.* **16**, 5410–5421 (2020).

[8] Zaverkin, V., Molpeceres, G. & Kästner, J. *Mon. Not. R. Astron. Soc., Submitted.*

[9] Schömig, R., Kästner, J. and Molpeceres, G. *In preparation.*