Quantum Chemical Simulations to Unveil the Interstellar Grain Surface Chemistry. Insights at an Atomistic Scale

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The Universe is molecularly rich [1]. Its chemical diversity and complexity is reflected by the more than 250 molecular species detected in the gaseous phase by means of radioastronomy [2] and the different solid-state phases in the form of dust grains [3]. The presence of the gas-phase molecules cannot be explained uniquely by reactions taking place in the gas phase but chemical reactions occurring on the surfaces of grains are essential to rationalize the interstellar chemistry. However, combining astronomical observations with astrochemical modelling and laboratory experiments is not enough to fully unveil the grain surface chemistry and its contribution to the chemistry of space because they hold some intrinsic limitations [4,5,6]. Quantum chemical simulations can partly alleviate this as they provide reliable, quantitative atomic-scale information (structure, energetics, and dynamics) of chemical processes taking place on the surface of grains, this way allowing us to determine the actual role of the grains on them, that is, as chemical catalysts, reactant concentrator and/or third bodies. This contribution aims to present some of the potentialities of current state-of-the-art computations developed in the *QuantumGrain* group to obtain unique and fundamental information that help improving our know-how on the grain surface chemistry. To this end, examples on the modelling of realistic grain surfaces for ices and silicates [7], on simulations dealing with the adsorption of astrochemically-relevant species [8] and with chemical reactions forming ethanol from CCH reacting with water ice [9], and finally on the fate of the extra energy released in an exothermic reaction (here the H_2 formation, [10]) will be presented.

References

[1] E.F. van Dishoeck, 2014, Farady Disc. 168, 9.
[2] B.A. McGuire, 2018, ApJS 239, 17.
[3] P. Ehrenfreund, & S.B. Charnley, 2000, ARA&A 38, 427.
[4] P. Caselli, & C. Ceccarelli, 2012, A&AR 20, 1.
[5] H.M. Cuppen, C. Walsh, T. Lamberts, et al., 2017, Space Sci. Rev. 212, 1.
[6] A. Potapov, & M. McCoustra 2021, Int. Rev. Phys. Chem. 40, 299.
[7] A. Rimola, S. Ferrero, A. Germain, M. Corno, & P. Ugliengo, 2021, Minerals 11, 26.
[8] S. Ferrero, L. Zamirro, C. Ceccarelli, A. Witzel, A. Rimola, & P. Ugliengo, 2020, ApJ 904, 11.
[9] J. Perrero, J. Enrique-Romero, B. Martínez-Bachs, et al., submitted to ACS Earth Space Chem.
[10] S. Pantaleone, J. Enrique-Romero, C. Ceccarelli, et al., 2021, ApJ 917, 49.