Capturing the Essence of Interstellar Icy Grains: Unveiling Computed Binding Energies and Frequency Distributions of Significant S-Bearing Species

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Binding energies (BEs) are crucial parameters to understand the evolution of molecular species in dense clouds, determining whether a species is frozen onto the grain surfaces or free in the gas phase. Nowadays, BEs are usually provided as single point values. However, the predominant amorphousness of icy grains gives rise to a distribution of BE sites and values. Until now, several grain models have appeared in literature, but they lack a comprehensive physical and systematical description. Recently, ACO-FROST, an automatic procedure to simulate realistic icy grains has been released.[1] This code allows us to build up models of amorphous ice up to 1,000 atoms and to simulate a large variety of BE sites (see Figure 1 – left panel).

In the present contribution, the aforementioned procedure was applied to compute BE distribution of high relevant S-bearing species, i.e., H_2S, OCS, CH_3SH. S-species were selected in order to contribute to a long-standing issue in the field: the sulphur depletion problem.[2] BEs were computed at DFT level (B97-3c) and then refined with one of the highest level of theory available (DLPNO- CCSD(T)). The previous reported BE values are overestimated with respect to our new BE distribution,[3] (see Figure 1 – central panel). Besides, frequency distribution was calculated for OCS molecule and compared to the James Webb Space Telescope (JWST) observations[4] (see Figure 1 – right panel). The computed distribution outstandingly reproduces JWST data indicating the robustness of the model studied and thus defining a novel computational tool to predict icy species vibrational features.

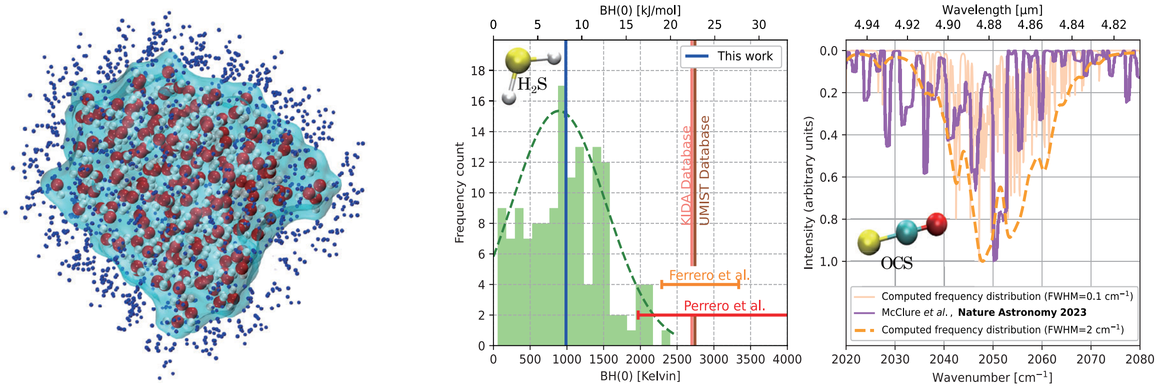

Figure 1: Left panel: 200-H_2O grain covered by a grid of 486 BE sampling sites. Central panel: BE distribution of H_2S compared with previous results. Right panel: Computed frequency distribution for OCS molecule compared with JWST observations.

References

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