Computational Study of Molecule-Ice Interactions in the Interstellar Medium

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Abstract

More than two hundred molecular species have been found in the interstellar medium (ISM). Study of the interactions of small molecules and radicals with dust grains carries paramount significance in our understanding of the formation of larger organic molecules found in the ISM and the astrochemical evolution of the ISM. We have computed the binding configurations and energies for 21 small molecules and radicals on crystalline ice surfaces using the density functional theory (DFT). We assessed the accuracy of our methods by comparing our results with available experimental evidence and previously published computational binding energies. Our results showed good agreement with results of higher level of theory.

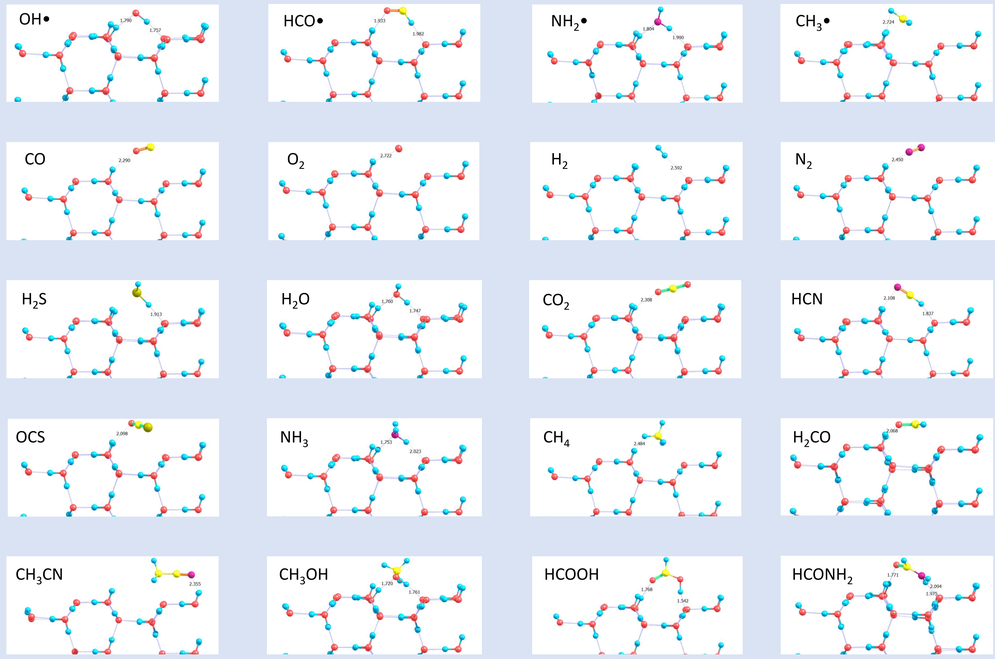
Why do this?

- First step in a larger project studying the formation of larger molecules in the interstellar medium (ISM)
- Understand how a selected group of small molecules and radicals interact with icy dust grains in the ISM
- Test the accuracy of our computational methods by comparing our results to previously published results

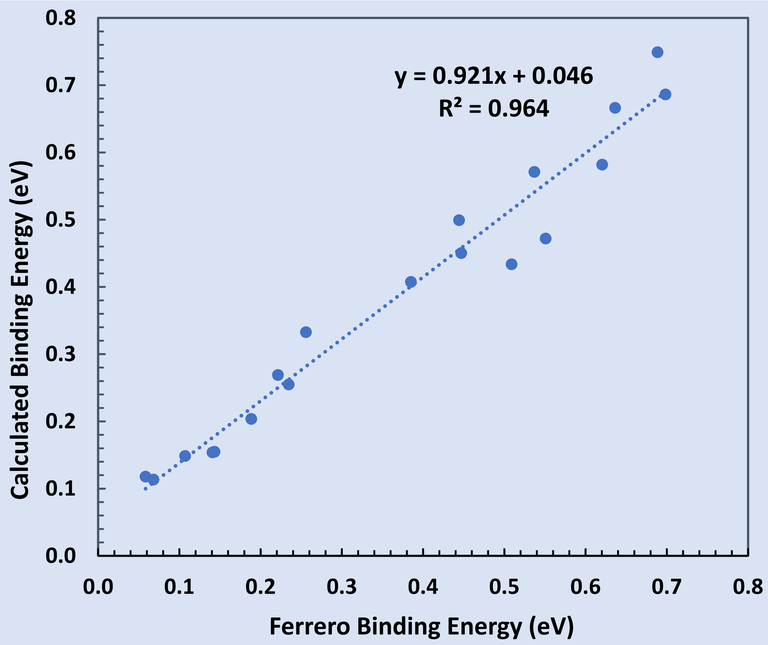
Methods

- Vienna Ab initio Simulation Package (VASP)
- Spin-polarized calculations
- PBE-D3 method of density functional theory
- PAW potential for core electrons and plane-wave basis sets for valence electrons
- A cubic supercell of 20 Å edge for isolated molecules and a orthonormal supercell 13.83×12.71×30.00 $Å^3$ for molecule-ice combined systems
- Convergence criteria: 10^{-6} eV for the total energy and 0.01 eV/Å for the forces on atoms
- Chemcraft for building and visualizing structures
- Scaling factor of 0.854 was used to account for vibrational energies

Optimized Molecule-Ice Structures



Comparison of Binding Energies



Binding energy $E_b = E_{mol} + E_{ice} - E_{mol-ice}$

Observations

- Free radicals took longer to optimize and calculate the binding energies due to the extra unpaired electron
- Initial placement of the molecule relative to the ice surface influenced final structure and binding energy
- Multiple initial configurations need to be explored in order to locate the lowest-energy structure
- Most molecules are physisorbed to the ice surface
- HCl dissociates when binding to the surface (different from Ferrero's report for crystalline ice)
- Clear linear relationship between VASP binding energy and Ferrero's results

Conclusions and Future Work

- Our results are fairly consistent with those published by Ferrero *et al*.
- The calculated binding energies correlate linearly with those reported by Ferrero et al.

$$E_b = 0.92\, E_{Ferrero} + 0.05$$

- This study will be extended to amorphous solid water (ASW)- a more realistic model for the dust grain mantle
- We can use this method to investigate the interaction between molecules found in the ISM and potential planetary surfaces like ice

References

- Ferrero et al. 2020, "Binding Energies of Interstellar Molecules on Crystalline and Amorphous Models of Water Ice by Ab Initio Calculations". The Astrophysical Journal **904,** 11.

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