



Universiteit
Leiden

The Netherlands

From adsorption to dissipation: insights from computer simulations of solid H₂O and CO

Ferrari, B.C.

Citation

Ferrari, B. C. (2026, June 10). *From adsorption to dissipation: insights from computer simulations of solid H₂O and CO*. Retrieved from <https://hdl.handle.net/1887/4304940>

Version: Publisher's Version

License: [Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/4304940>

Note: To cite this publication please use the final published version (if applicable).

Propositions

accompanying the thesis

From Adsorption to Dissipation: Insights from Computer Simulations of Solid H₂O and CO

1. The Julia programming language enables us to develop highly performant code that is also easy to use (Chapter 3).
2. Highly ordered ice Ih (0001) surfaces can produce binding sites with binding energies higher than the cohesive energy of the ice crystal (Chapter 4).
3. CO binding on CO clusters is dominated by dispersion and depends on the size of the cluster (Chapter 5).
4. Vibrationally excited CO molecules in solid CO primarily redistribute their energy via vibrational-vibrational energy transfer (Chapter 6).
5. Modern many-body potentials for water are as accurate as high-level *ab initio* calculations, while also being significantly less computationally demanding. This makes them the best choice for studying water (Zhu, Xuanyu, *et al.* *Journal of Chemical Theory and Computation* 19.12 (2023): 3551-3566).
6. When dealing with systems that contain disorder, a less accurate method that allows for more sampling is the best method (Batista, Enrique R., and Hannes Jónsson. *Computational materials science* 20.3-4 (2001): 325-336).
7. Proprietary scientific software is detrimental to modern science. (Ramachandran, Rahul, Kaylin Bugbee, and Kevin Murphy. *Earth and Space Science* 8.5 (2021): e2020EA001562).
8. Proper software engineering practices are vital to healthy scientific software. Unfortunately, the “publish or perish” system in academia actively discourages these practices. (Heaton, Dustin, and Jeffrey C. Carver. *Information and Software Technology* 67 (2015): 207-219).
9. Where you are born says nothing about you as a person.

Brian C. Ferrari
Leiden, 10 June 2026