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

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chapter research grant. This was a small grant for students to carry out independent research style projects. I was awarded $ 2,000 to build an experimental setup for performing the Cavendish experiment to measure the gravitational constant. Upon completion of this project, it was incorporated into the undergraduate UCF physics laboratory course for physics majors.

As an undergraduate student I joined a research group, another recommendation from Costas, headed by Dr. Christopher J. Bennett at UCF. At this point I had worked for a year as a machinist apprentice, so I was able to construct an ultrahigh vacuum (UHV) in Chris's laboratory, as well as design and machine a custom-made sample holder and various subsequent variants for the chamber. Alongside the laboratory work, I began running computational calculations of astrophysically relevant molecules. Upon completing my bachelor's degree, I accepted a PhD position at UCF to continue working under Chris. It was during this time that I met my wife, Katie Slavicinska, who a semester after me also accepted a PhD position in the Bennett lab.

At the time, the American science funding was orders of magnitude ahead of the world, and so it was common for PhD students to apply for grants. Chris advised me to apply for various NASA grants and fellowships. I managed to secure a $ 165,000 NASA fellowship and an additional $ 4,000 research grant. The NASA fellowship was a joint NASA Ames and UCF research project where I was supposed to spend summers at NASA Ames. Unfortunately, COVID prevented me from going to NASA Ames my first year, and shortly after that, I left UCF.

In search of better PhD prospects, my wife and I applied for two positions in the Leiden Laboratory for Astrophysics. Unfortunately, only one position was available, but it was made clear to us that another faculty member at Leiden University was looking for a PhD student. The other faculty member, Thanja Lamberts, worked in theoretical chemistry, meaning only I was qualified for the position.

At Leiden I worked under Thanja for the first few years, then transitioned to working under Jörg Meyer for the remaining time. April 20^{th}, 2023 I completed a course on scientific conduct at the Graduate School of Science. My PhD work has culminated in a handful of publications. However, what I'm truly proud to have produced during my PhD is my Julia package *YetAnotherSimulationSuite.jl*.

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Data Availability

Chapter 5

All of the Python code used for the simulations is publicly available on GitHub at https://github.com/Cavenfish/CO_Project. XYZ files for all clusters used in this work can be found on Zenodo at https://zenodo.org/records/8068393.

Chapter 6

All of the Julia code used for the simulations is publicly available on GitHub at https://github.com/Cavenfish/YetAnotherSimulationSuite.jl. An HDF5 compliant dataset (Julia Data Format ".jld2") of all ensemble averages reported within the manuscript can be found on Zenodo at https://zenodo.org/records/14237514.