# Nuclear quantum effects in solid water: new insights from computational modeling

Rasti, S.

## Curriculum Vitae

Soroush Rasti was born on the 2$^{nd}$ of August 1991 in Isfahan (Iran). From 2003 to 2009, he followed his pre-university educations in his hometown. He received his B.Sc. degree in Physics in 2012 from the University of Tehran *cum laude* with the highest total GPA 18.37 among this classmates. In the last year of his bachelor studies, he participated in the National Physics Olympiad and obtained the 5$^{th}$ rank. After that in 2014, he entered Sharif University of Technology exceptionally without entrance exam as a brilliant young talented student. He received his Physics M.Sc. degree in 2015 *cum laude* again with the highest total GPA 19.37 among his classmates. After his master study, he did an internship in Japan in the molecular science department of the National Institute of Natural Science under the supervision of Prof. dr. K. Ohmori. This research was about developing a new type of Rydberg quantum simulators and computers. After that, Soroush joined the group of Dr. P. Kaghazchi at the Free University of Berlin as a visitor to perform research for the next generation of batteries focusing on the molecular level. In October 2016, Soroush started his PhD research under the supervision of Dr. Jörg Meyer at the in the theoretical chemistry group (headed by Prof. dr. Geert-Jan Kroes) of the Leiden Institute of Chemistry. His research was funded by the Netherlands Organisation for Scientific Research (NWO) and led to this thesis. From August 2021 onward, Soroush is working as a data science leader in a company focused on developing a new marketing model using artificial intelligence.

## List of Publications

- S. Rasti and J. Meyer, Importance of zero-point energy for crystalline ice phases: A comparison of force fields and density functional theory, *J. Chem. Phys.* **150**, 234504 (2019).
- V. Fuentes-Landete, S. Rasti, R. Schlögl, J. Meyer and T. Loerting, Calorimetric Signature of Deuterated Ice II: Turning an Endotherm to an Exotherm, *J. Phys. Chem. Lett.* **11**, 8268 (2020).
- E. Ö. Jónsson, S. Rasti, M. Galynska, J. Meyer and H. Jónsson, Transferable Potential Function for Flexible $H_2O$ Molecules Based on the Single Center Multipole Expansion, *submitted to the Journal of Chemical Theory and Computation (JCTC)*
- S. Rasti, E. Ö. Jónsson, H. Jónsson and J. Meyer, New Insights into the Volume Isotope Effect of Ice Ih from polarizable many-body Potentials, *to be submitted*

## Afterword

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