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

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Curriculum Vitae

Soroush Rasti was born on the 2nd 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 5th 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 H₂O 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

Finally, my long academic journey as PhD student has been finished. It was full of all sorts of happiness, frustration, anxiety, hope and all other kinds of overwhelming emotions. I would like to thank the many people without whom I would not have finished this hard but enjoyable journey, and without whom I would not have been able to complete this research.

First, I would like to thank my PhD advisor **Jörg Meyer** for giving me the chance to pursue my PhD career at Leiden University and being patience and supportive during my doctoral research. His supportive approach and way of working helped me to develop some skills that allowed me to improve the quality of my work. In addition, I like to especially appreciate the tremendous time and effort he spent on proofreading the papers and this thesis: this thesis would not have been completed without your help and guidance. I am also thankful to my promotor **Geert-Jan Kroes** for generously sharing his priceless wisdom and experience with me.

I am very grateful to have been a part of the Leiden Theoretical Chemistry group, where I worked with many good colleagues. My special thanks to **Khosrow Shakouri** and **Hossein Tahmasbi** for helping me a lot in every moment of my PhD as a daily supervisor. I feel very lucky to have such exceptional friends. I never forget your encouragements and pleasing words about being perseverant and not to give up. I am thankful to **Thanja Lamberts** for teaching me how to supervise bachelor projects and being available for my questions. Thank you **Mark Somers** and **Marc van Hemert** for your advice about my presentations in the group. I also enjoyed being

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