

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

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Propositions

accompanying the thesis

"Nuclear Quantum Effects in Solid Water – New Insights from Computational Modeling"

- (i) Many-body force fields based on sophisticated parametrization schemes prove more successful than density functional theory with currently available exchange-correlation functionals when it comes to modelling properties of water ice (Chapters 3 and 6).
- (ii) When developing or refining a general-purpose interaction potential for water, nuclear quantum effects for vibrations should be taken into account – at least at the level of zeropoint energy (Chapter 5).
- (iii) More experimental data for frequency shifts upon compression and expansion of ice will help to benchmark and

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further improve the accuracy of computational models for water ice and thus our understanding of nuclear quantum effects therein (Chapter 6).

- (iv) Including a description of vibrational properties at the quantum mechanical level can have a big influence on thermodynamical properties of crystalline phases of condensed water (Chapters 3, 4, 5 and 6).
- (v) Quantitative modelling of nuclear quantum effects in ice and other materials still requires improvements of the accuracy of computational models.
- (vi) A method that predicts an approximate value for the right reason is more valuable than a method that predicts the same value more accurately but for the wrong reason (e.g., error cancellation).
- (vii) The development of a theoretical or computational method itself is very insightful even if the results obtained with it fail to describe experimental data correctly.
- (viii) Research in fundamental science such as theoretical chemistry needs long-term funding.
- (ix) A course about critical thinking and reasonable argumentation should be part of a PhD programme.
- (x) If you have a PhD, it is not the lack of specific technical skills that prevents you from getting a business job, but the lack of communication and networking with people not having a PhD.
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