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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 zero-point energy (Chapter 5).
- (iii) More experimental data for frequency shifts upon compression and expansion of ice will help to benchmark and

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.