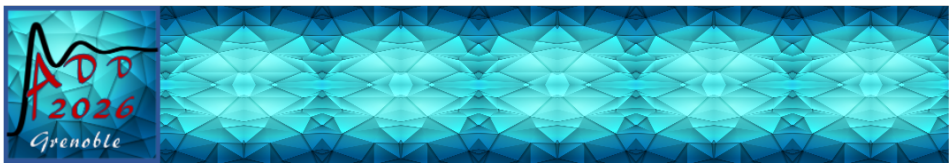

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Hidden complexity in D2O Ice VII

Content

Ice VII is thought to play a role in the water-rich interiors of Jupiter's moon Europa and Saturn's moon Enceladus and other planetary bodies. From its average cubic structure, ice VII is seemingly simple, however the local structure reveals hidden complexity, namely individual positions of water molecules forming a complex network via hydrogen bonds. Through coupling Pair Distribution Function and Reverse Monte Carlo modelling to high pressure neutron scattering data, we have quantified the atomic and molecular structures of disordered ice VII. The decomposition of the average structure of ice VII into the individual positions of water molecules within the crystal lattice reveals that the D2O molecules are displaced along the direction of the polarization vector of each molecule. By applying this displacement, the structural model more accurately matches the D–O distances and D–O–D angles determined from the other ordered ice structures. Our results are also supported by DFT calculations confirming that deviations of water molecules from their average crystallographic positions energetically stabilize the structure of ice VII. Our studies open new perspectives for structural studies of different forms of ice, their phase transitions treating them as vast clusters of molecules with an average periodic structure but symmetry-free local arrangements.

Primary authors: SLAWINSKI, Wojciech (Univeristy of Warsaw, Faculty of Chemistry); Prof. WOZNIAK, Krzysztof (University of Warsaw)

Co-authors: Dr ARHANGELSKIS, Mihails (University of Warsaw); Prof. BULL, Craig (Rutherford Appleton Laboratory ISIS Neutron and Muon Source); Dr CHODKIEWICZ, Michal (University of Warsaw); Dr GAJDA, Roman (University of Warsaw); Dr LACH, Grzegorz (University of Warsaw); Dr REJNHARDT, Piotr (University of Warsaw); Dr RIDLEY, Christopher (Oak Ridge National Laboratory)

Presenter: SLAWINSKI, Wojciech (Univeristy of Warsaw, Faculty of Chemistry)

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Submitted by **SLAWINSKI, Wojciech** on **Friday, November 7, 2025**