| Participants: | Mikael Leetmaa and Thor Wikfeldt from Stockholm University |
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| Contribution: | One poster |
| Title: | Studying the structure of water with RMC by incorporating constraints from various experimental techniques |

Abstract

In light of the ongoing debate regarding the structure of liquid water, structural models of water have been created with the RMC method with the aim of satisfying as many experimental constraints as possible. Apart from fitting to recent X-ray and neutron diffraction data, experimental observations from X-ray absorption spectroscopy (XAS) have been incorporated into the fits in the form of geometrical constraints. In order to obtain structures fulfilling the geometrical requirements observed in XAS data, angularly resolved coordination constraints have been implemented in the RMC++ code. Additionally, the use of an intermolecular potential has also been implemented in the code to avoid certain unphysical structures.