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(POS-12) The influence of dynamic/tetrahedral correlations on the ice/water interface

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Understanding the mechanisms present behind ice growth in a system of liquid water has posed many challenges, primarily due to the difficulties associated with simulating and quantifying these behaviours microscopically. Here, we make use of previously established molecular dynamics methodologies with the express goal of simulating the steady state growth and melting of ice. The standard TIP4P water model is used to represent the (001) face of cubic ice, and various temperature gradients centered about the melting temperature are applied to ensure proper ice/water coexistence. We investigate the dependency of ice growth and melting on the presence of tetrahedral and dynamic heterogeneities in liquid water. This is done using the isoconfigurational ensemble to identify clusters of tetrahedrally ordered and disordered molecules and clusters of molecules exhibiting fast and slow dynamics. It has been previously observed that crystalline precursor structures in liquid water correlate with regions with regions of slow dynamics and that the presence of dynamic and tetrahedral heterogeneities have a strong effect on the system's behaviour. Therefore, we seek to explore the role these regions play in ice growth and melting, and how tetrahedrally ordered and disordered clusters of molecules may influence where these regions form.

Keyword-1

molecular dynamics simulations

Keyword-2

ice crystal growth

Keyword-3

Author: MUISE, Mathieu (Memorial University)

Co-authors: Dr SAIKA-VOIVOD, Ivan (Memorial University); Dr RAZUL, M. Shajahan (St. Francis Xavier University)

Presenter: MUISE, Mathieu (Memorial University)

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