The Role of Tetrahedral Order in Dynamical Heterogeneity in Supercooled Water

M **Shajahan G Razul**[1]*, Gurpreet S Matharoo[2,3†] and Balakrishnan Viswanathan[4‡]

[1] Department of Chemistry, St. Francis Xavier University, Antigonish, NS, B2G 2W5, Canada.
[2] ACENET, St. Francis Xavier University, Antigonish, NS, B2G 2W5, Canada.
[3] Department of Physics, St. Francis Xavier University, Antigonish, NS, B2G 2W5, Canada.
[4]Quest University, Squamish, BC,V8B 0N8, Canada.

***sgrazul@stfx.ca (Corresponding author)**

† **gmatharo@stfx.ca**

‡ **bviswana@stfx.ca**

ABSTRACT

In this study we use Molecular Dynamics simulations in the isoconfigurational (IC) ensemble to investigate the supercooled state of SPC/E water of multiple starting configurations at three different temperatures to discover the connection between emerging heterogeneities in the tetrahedral order parameter and the dynamic propensity. Here, we investigate the connection between structure (particularly the tetrahedral structure) and dynamics of water. Furthermore, the use of tetrahedral order will be used to identify crystalline environments and we can probe the connections between crystal-like particles and dynamical heterogeneity in water. We aim to show that heterogeneities of the tetrahedral order parameter exist, where the spatial regions of high and low tetrahedral order exist and are linked to the underlying dynamical heterogeneity, as opposed to being random and scattered evenly (spatially) throughout the system. We thus employ the IC ensemble to uncover the properties of this water system to highlight its utility as a tool and for the important structural and dynamical insights it can provide beyond single configurations.