Unlocking the Mysteries of Supercooled Water: Translational Jump-Diffusion Approach in Explaining the Dynamical Anomalies

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Despite being the most ubiquitous liquid, water exhibits numerous thermodynamic and dynamic anomalies, which intensify in its supercooled state. While thermodynamic anomalies have been extensively studied, dynamical anomalies have received less attention due to the experimental challenges involved. One significant dynamical anomaly is the violation of the Stokes-Einstein relation (SER), which connects particle diffusion to the medium's viscosity.[1-3] Although some theories have attempted to explain this breakdown, a detailed molecular mechanism remained elusive.[4] Our group has developed the Translational Jump-Diffusion (TJD) approach, which successfully explains the SER breakdown in supercooled water and aqueous solutions.[5-8] We have discovered that the increasing contribution of translational jumps to total diffusion is responsible for the diffusion-viscosity decoupling observed in these systems. Based on this approach we have developed a theoretical method to compute the micro-viscosity of water in nanochannels and other complex confined environments.[9-10] These findings hold significant promise for elucidating various dynamical anomalies in bulk supercooled water and water under confinement.

References

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