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# Water as a Solvent through Static and Dynamic Calculations : A Theoretical Perspective

**Dhivya Manogaran**
*Indian Institute of Science Bangalore, India*

The talk discusses water as a solvent at the molecular level using a combined Quantum Chemical and Molecular Dynamics approach. The presentation focusses on the making and breaking of Hydrogen bonds through an analysis of the Hydrogen bond correlation functions computed from the molecular trajectories and the Hydrogen Bond Strength based on interaction coordinates derived from the Cartesian force constant matrix. The Translational-Rotational motion coupling in liquid water is elucidated using a simplistic approach of variable mass effects induced deviation from the Stokes-Einstein behavior in model water systems. Several noted interesting trends and key factors determining the solution dynamics are discussed.

## Biography

Dhivya Manogaran did her PhD in theoretical chemistry at University of Texas at Austin and a postdoc at Indian Institute of Science Bangalore. She has published 13 papers in widely read international journals and hopes to continue making significant contributions to the field.