TIFR Centre for Interdisciplinary Sciences
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Seminar

The effect of quantum nuclear motion on hydrogen bonding

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Most of chemistry can be understood by treating the atoms in molecules as classical particles. Quantum zero-point motion and tunnelling do not play a key role. Important exceptions are molecules involving hydrogen bonding, including water, proton sponges, organic acids, and some enzymes. Quantum nuclear effects are revealed by isotope substitution experiments where hydrogen is replaced by deuterium. I will introduce a simple model for hydrogen bonding [1] based on a two-dimensional electronic Hilbert space that gives potential energy surfaces that can be used to calculate the quantum vibrational states of the shared proton/deuterium. This leads to a quantitative description of experimental data for bond lengths, vibrational frequencies, and isotope effects for a diverse range of chemical compounds [2].

[1] R.H. McKenzie, Chem. Phys. Lett. 535, 196 (2012).
[2] R.H. McKenzie, C. Bekker, B. Athokpam, and S.G. Ramesh, J. Chem. Phys. 140, 174508 (2014).

Wednesday, Nov 12th 2014

4:00 PM (Tea/Coffee at 3:30 PM)

Seminar Hall, TCIS