

Intermolecular hydrogen bonds: From temperature-driven proton transfer in molecular crystals to denaturation of DNA

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Abstract. We have combined neutron scattering and a range of numerical simulations to study hydrogen bonds in condensed matter. Two examples from a recent thesis will be presented. The first concerns proton transfer with increasing temperature in short intermolecular hydrogen bonds [1,2]. These bonds have unique physical and chemical properties and are thought to play a fundamental role in processes like enzymatic catalysis. By combining elastic and inelastic neutron scattering results with *ab initio*, lattice dynamics and molecular dynamics simulations, low frequency lattice modes are identified which modulate the potential energy surface of the hydrogen bond proton and drive proton transfer.

The second example concerns base-pair opening in DNA which is the fundamental physical process underlying biological processes like denaturation and transcription. We have used an empirical force field and a large scale, all-atom phonon calculation to gain insight into the base-pair opening modes and the apparent ‘energy gap’ between the accepted frequencies for these modes ($\sim 100\text{ cm}^{-1}$ or $\sim 140\text{ K}$) and the temperature of the biological processes (room temperature to 100°C) [3]. Inelastic neutron scattering spectra on aligned, highly crystalline DNA samples, produced at the ILL, provide the reference data for evaluating the precision of these simulation results.

Keywords. Neutron scattering; dynamics.

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References

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