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**Research Interests: computational chemistry, density functional theory, molecular dynamics, molecular crystals, hydrogen bonding (proton migration and transport).**



When experimental methods yield only partial results it is the role of theory to complete the story. The central aim of our research group is to exploit the synergistic relationship that now exists between computation and experiment.

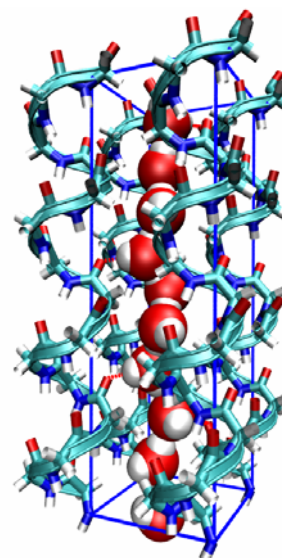


Much of our research evolves around protons in molecular structures: this could involve accurately locating their positions in high temperature and pressure X-ray diffraction studies, or studying their motion using molecular dynamics simulations. Our interests here include fitting anharmonic probability distributions to better describe vibrations of molecules in the solid state (see Figure left), as well as deriving mechanisms for proton migration and proton transport reactions.

We have recently reported *ab initio* MD simulations on a water wire embedded in an alpha-helical pore (see Figure right). This is a greatly simplified model for membrane-bound proteins, which are responsible for transporting protons into and out of cells, thereby controlling cell pH and energy production.

Our simulations focused on the mechanism by which an excess proton is able to travel along a chain of water molecules supported by the alpha-helical scaffold. Our results showed that, whilst the mechanism of proton transport shares many similarities with simulations performed on bulk water, there are important differences.

Other research interests in the group include modelling metal organic framework materials, which find application in hydrogen storage.



## SELECTED RECENT PUBLICATIONS

1. Using molecular dynamics simulations to understand and improve the treatment of anharmonic vibrations. II Developing and assessing new Debye-Waller factors. A. M. Reilly, K. R. McLean, C. A. Morrison and D. W. H. Rankin, *Acta. Cryst.* 2011, **A67**, 346.
2. Simulating proton transport through a simplified model of a trans-membrane protein. L.M.S. Shepherd and C. A. Morrison, *J. Phys. Chem. B.* 2010, **114**, 7047.
3. Investigating anharmonicity using molecular dynamics calculations: the TM hydride series  $(\text{PH}_3)_3\text{MH}_4$ , (M = Os, Ru and Fe). C. A. Morrison and A. M. Reilly, *Dalton Trans.* 2010, **39**, 5527.
4. Temperature and Pressure-induced Proton Transfer in the 1:1 Adduct formed between Squaric Acid and 4,4'-Bipyridine. D. M. S. Martins, D. S. Middlemiss, C. R. Pulham, C. C. Wilson, M. T. Weller, P. F. Henry, N. Shankland, K. Shankland, W. G. Marshall, R. M. Ibberson, S. Moggach, M. Brunelli and C. A. Morrison, *J. Am. Chem. Soc.*, 2009, **131**, 3884.