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Research keywords: Excited State Dynamics, Quantum Dynamics, Molecular Dynamics, Energy and Electron transfer, X-ray Spectroscopy.

Research in my group focused upon computational and theoretical chemistry to deliver detailed understanding of non-equilibrium molecular and materials properties. The research interests of the group are focused upon developing methods for and understanding excited state properties, nonadiabatic ultrafast dynamics and time-resolved spectroscopy. We have strong expertise in X-ray spectroscopy and molecular dynamics. Through the North East Centre of Energy Materials (NECEM) project, we are studying charge transfer across interfaces. This includes detailed studies into the coupled nuclear and electronic dynamics associated with electron transfer into polyoxometalates.

References

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- [4] G. Capano, C.J. Milne M. Chergui, U. Rothlisberger, I.Tavernelli and T.J. Penfold* Probing Wavepacket Dynamics using Ultrafast X-ray Spectroscopy. J. Phys. B **48**:214001 (2015).