Simulating Linear and Nonlinear Spectroscopies of Aqueous Systems

Vibrational spectroscopy (e.g. infrared, Raman) is a standard approach to characterise molecular and material systems via their vibrational modes. Generally, a wide range of experiments are brought to bear on a system and several different kinds of spectra are measured, giving information on the structure and dynamics of a material as well as the mechanisms of energy transfer and its symmetry. This results in a large amount of information that may be difficult to disentangle.

To help with this, it is common nowadays to use computer simulations to help interpret experimental results, but these simulations come with their own problems: highly accurate quantum-mechanical calculations are needed not only for the dynamics of the system but also for its response to the electric field of light. The level of accuracy needed renders these calculations completely intractable. However, over the past few years my research team has shown that it is possible to use machine-learning methods to completely circumvent these calculations, paving the way to predict vibrational spectra easily and accurately.

In this project, you will build state-of-the-art machine-learning models for the energies, forces and electric responses of electrolyte solutions and of water-mineral interfaces, and use these, along with imaginary-time path-integral methods, to simulate the results of vibrational spectroscopy on these systems. I have collaborators with research groups in Switzerland and the US who are interested in comparing their experiments with simulations, and this project will provide opportunities for international collaboration.

For informal inquiries, please feel free to contact Dr. David Wilkins (d.wilkins@qub.ac.uk) at the Centre for Quantum Materials & Technologies, School of Mathematics & Physics, Queen's University Belfast.

Entry requirements

Applicants are expected to possess a first or upper-second class degree in physics, chemistry, materials science, or a relevant discipline (or an equivalent overseas qualification), or a lower second-class degree along with a Master's degree.

How to apply

Applications should be submitted via the Direct Applications Portal.

References

1. V. L. Deringer et al., *Chem. Rev.* **121**, 10073 (2021)
2. S. Shepherd, J. Lan, D. M. Wilkins, V. Kapil, *J. Phys. Chem. Lett.* **12**, 9108 (2021)
3. S. Shepherd, G. A. Tribello, D. M. Wilkins, *J. Chem. Phys.* **158**, 204704 (2023)
4. Y. Litman, J. Lan, Y. Nagata, D. M. Wilkins, *J. Phys. Chem. Lett.* **14**, 8175 (2023)