Vibrational Spectroscopy for Water Treatment

A lot of research in modern environmental science is not about preventing future harm, but in reckoning with and mitigating against harm already done by humans. The by-products of manufacturing processes thought originally to be harmless have turned out to be dangerous to human and wildlife health. One key example is so-called “forever chemicals”, which are used in making a huge variety of products. These chemicals persist in the environment and are very hard to remove. To understand how best to get forever chemicals out of the drinking supply, we need to understand their properties in as much detail as possible.

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. To help disentangle the large amount of information gained from these experiments, it is common nowadays to use computer simulations to help interpret experimental results.

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. This project will leverage state-of-the-art machine-learning models with atomistic simulations to predict vibrational spectra for emerging contaminants.

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. S. Shepherd, G. A. Tribello, D. M. Wilkins, *J. Chem. Phys.* **158**, 204704 (2023)
2. Y. Litman, J. Lan, Y. Nagata, D. M. Wilkins, *J. Phys. Chem. Lett.* **14**, 8175 (2023)
3. A. Jana, S. Shepherd, Y. Litman, D. M. Wilkins, *J. Chem. Inf. Model.* **64**, 4426 (2024)