Experiment vs. Theory: An Empirical Assessment of Computational Interaction Energies in Solution

A PhD studentship is available in the group of Prof. Scott Cockroft, School of Chemistry, The University of Edinburgh; https://www.cockroft.chem.ed.ac.uk
The studentship is fully funded for 42 months by the University of Edinburgh and covers tuition fees and an annual stipend (starting at £18,622 per annum) for a candidate satisfying EPSRC residency criteria. https://www.ukri.org/councils/esrc/career-and-skills-development/funding-for-postgraduate-training/eligibility-for-studentship-funding/#contents-list

Project Summary
A multitude of computational methods exist for assessing the strength of non-covalent interactions, including newer methods for assessing London dispersion. Meanwhile, experimental measurements in solution are now beginning to reveal the significance of dispersion interactions. However, the accurate computational prediction of competitive solvation energetics remains elusive. Perhaps surprisingly, our preliminary comparisons reveal that older computational methods provide better energetic predictions of experimental data than modern dispersion-corrected methods. We will use extensive data collected by the Cockroft group and the broader literature to seek the correct "blend" of computational methods that make the best empirical predictions of interactions energies in solution. The applicant or other Cockroft group members (depending on expertise) will synthesise new model compounds to test predictions and fill the gaps in existing experimental knowledge.

In the first instance, the initial application (including cover letter and CV) should be directed to:
Prof. Scott Cockroft, School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK. scott.cockroft@ed.ac.uk

The position will remain open until filled; prompt applications are encouraged.

References
Context-dependent significance of London dispersion, L. A. Gravillier, S. L. Cockroft, *Acc. Chem. Res.*, 2023, DOI: 10.1021/acs.accounts.3c00625

IMPORTANT
Before Submitting your cover letter and CV, please complete the online School of Chemistry Equality, Diversity and Inclusion Form 2024.

The form will automatically generate a unique "Receipt Number" that you MUST include in your cover letter.

Equality and Diversity
The School of Chemistry holds a Silver Athena SWAN award in recognition of our commitment to advance gender equality in higher education. The University is a member of the Race Equality Charter and is a Stonewall Scotland Diversity Champion, actively promoting LGBT equality. The University has a range of initiatives to support a family friendly working environment. See our University Initiatives website for further information. University Initiatives website: https://www.ed.ac.uk/equality-diversity/help-advice/family-friendly