Context: Spin-coupled valence bond (SC VB) theory is a quantum-chemical approach which uses a compact high-quality wavefunction to achieve easy-to-interpret descriptions of chemical bonding. In addition to providing one of the most popular models for the electronic structure of benzene, SC VB theory has been used to obtain a number of new, interesting and often unexpected insights into the electronic mechanisms of wide range of organic reactions, including the Diels-Alder reaction, the Cope rearrangement, electrocyclisation reactions, the 1,3-dipolar additions, etc.

Project: We have recently developed an extension of SC VB theory which allows its application to molecular systems in which the number of important (or ‘active’) electrons is different from the number of orbitals which accommodate these electrons. Examples include ions and molecules containing hypervalent atoms. The aim of this project is to apply extended SC VB theory to a series of molecular systems and chemical reactions which we have not been able to study with the older, ‘traditional’ version of the SC VB approach. These include Möbius cycles such as C₉H₉⁺ which attract considerable synthetic interest, and are considered as 4n-aromatic, 1,3-dipoles such as diazomethanes and their reactions.

Background: The three references listed below provide information about the theoretical background of the project and examples of the applications of SC VB theory to chemical structure and reactivity.

Research Group: The student will join a small but vibrant quantum chemistry research group that develops new computational methods and applies these to a range of molecular systems and chemical reactions.

Training will be provided in quantum chemistry and the use of computers for quantum-chemical calculations. This includes the use of modern ab initio packages such as GAUSSIAN and GAMESS-US to calculate single-point energies and optimize geometries at various levels of theory, as well as our own SC codes. There is an opportunity to take part in method development and gain experience with writing scientific codes in Fortran. Students are expected to present their research findings at conferences. Opportunities exist for collaborative visits to other research groups in the UK and abroad.

Relevant Publications:


Eligibility: UK/EU/Overseas
Funding Types: Self-funding

For more information contact chemgrad@york.ac.uk or see our web page: http://www.york.ac.uk/chemistry/postgraduate

The Department of Chemistry holds an Athena SWAN Gold Award and is committed to supporting equality and diversity for all staff and students.