Research Associate in Theoretical Chemistry

Cardiff School of Chemistry

Cardiff University (UK)

We seek to recruit an enthusiastic, highly motivated scientist with proven intellectual and technical abilities to work on project in computational molecular quantum mechanics. The 2-year project, funded by the Leverhulme Trust, aims to develop a new computational framework for analysing the outcome of an accurate electronic structure calculation in terms of quantities related to the traditional conceptual models such as curved arrows and frontier orbitals.

The project builds on the standard computational methodology for determining molecular electronic structure. New theory, and software that implements it, will be created to take the outcome of such calculations - molecular orbitals, electron pair correlation functions, and the underlying hamiltonian operator that determines them - and analyse them by characterising key molecular orbitals and their changes along a reaction coordinate.

The post is available from 1 September, and is currently advertised at http://bit.ly/7230BR, with a closing date of 17th May. Informal enquiries (KnowlesPJ@Cardiff.ac.uk) are very welcome.