IT Services

Case Study

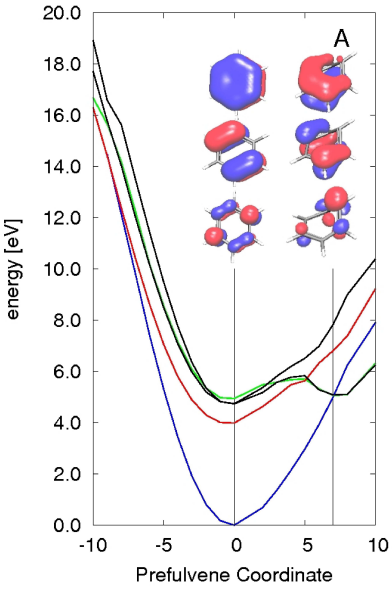
BlueBEAR provides a substantial computing resource that properly supports the research work of research staff and students at Birmingham. It provides a cost effective facility that optimises the effectiveness of research and ensures the University continues to be a world-class academic learning and research environment.

Femtochemistry

Challenges

We are investigating what happens to a molecule in the first few hundred femtoseconds after it absorbs a photon of light. This is the time period of molecular vibrations and can be tracked experimentally using very short pulses of laser light in what the Nobel prize winner Ahmed Zewail called ``femtochemistry'' experiments.

One example we have been studying, in collaboration with an experimental group at UCL, is benzene. After excitation, the energy can flow down various competing pathways and the interpretation of the experimental results is difficult.



Background

To study these systems using computer simulations we need to solve the time-dependent Schroedinger equation to follow the system wave function. For this we have an in-house code, the MCTDH program. First, we need to calculate the potential energy surfaces of all the electronic states involved. This can be done using standard quantum chemistry programs: we use Molpro and Gaussian. The energies need to be calculated at many thousand molecular geometries, for which BlueBear has been an essential tool. Once the potential surfaces are known we use the MCTDH program to follow the process we are modelling. Again these calculations need significant computer resources

Results

In benzene we were able to understand the energy flow observed in terms of competition between two main initial pathways. The figure shows a cut through the potential surfaces along a particular distortion of benzene. Initial excitation takes place to the green state (S1). From there it can flow and energy transfer to the other states where the curves cross if there is coupling between the states. Our simulations fitted the experiments very nicely and we showed that the triplet states (in black and red) play a significant role in the process, which is surprising as the coupling to the S1 state is tiny.

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Product Used
Molpro
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