

Quantum chemistry applied to electron driven processes

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Electron driven chemistry is important in a variety of processes in chemistry, biology and astrochemistry. Anion resonances are formed as metastable intermediates in low-energy electron-induced reactions. Due to the finite lifetimes of resonances a proper description requires obtaining both the energy and the lifetime (width) of the states. We have developed an approach that combines multireference methods with complex absorbing potentials (CAP-MRCI) in order to describe the energies and lifetimes of a variety of resonances, including Feshbach resonances, which are difficult to describe with single reference methods. The method has been tested in a variety of systems yielding good performance. We find that CAP-MRCI can efficiently capture the mixing between Feshbach and shape resonances, which is a very challenging issue. One of the applications that we are particularly interested in is the interaction of low-energy electrons with nucleobases which can lead to damage of nucleic acids. To gain understanding and accurately model electron damage in such systems we need to investigate electron attachment to nucleobases in the gas as well as in solvated phases. In order to do that we have also explored the effect of microsolvation/solvation on both resonances and dipole bound states in nucleobases.