**Nonorthogonal Configuration Interaction for the Calculation of Electronic Couplings**

R. Broer, L.E. Aguilar Suarez, R.K. Kathir, T.P.Straatsma, S. Faraji, R.W.A. Havenith

University of Groningen

r.w.a.havenith@rug.nl

**Abstract**

In singlet fission, the energy of a molecule in one of its excited states is split over two molecules, each then being in their first triplet state. This process can adequately be described in ensembles of molecules in terms of molecular states. For this purpose, we have developed a non-orthogonal configuration interaction method that allows the description of a molecular crystal, using the (embedded) cluster approach, in terms of many-electron basis functions (MEBFs), each describing a particular electronic state of a molecule in the ensemble. The MEBFs can be constructed as combinations of antisymmetrised products of molecular wavefunctions of the MCSCF-type. The advantage of this approach is that we can calculate the diabatic excited states in the ensemble, and the coupling between excited states localised on different molecules, such as the electronic coupling matrix element relevant for singet fission. In this poster, an overview of the method will be given.