CFEL SCIENCE

Colloquium

31st May 2013 – 14:00
CFEL bldg. 99 , seminar rooms I-III

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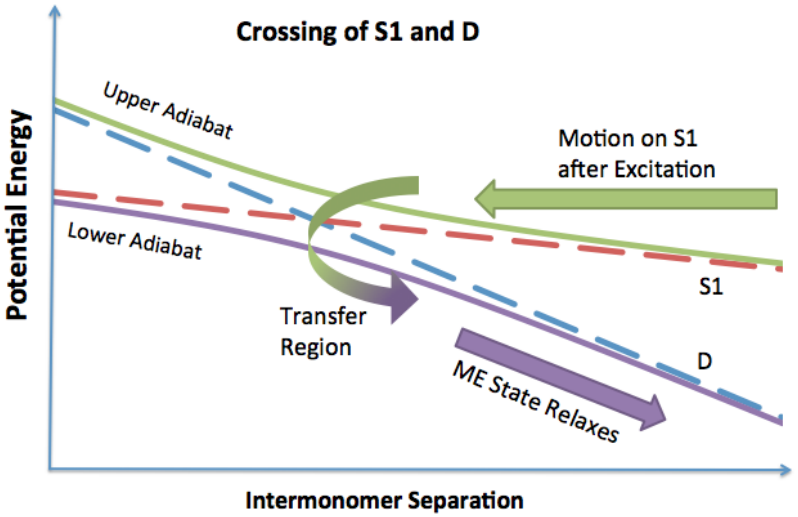
Electronic structure for excited states of strongly correlated molecules: Methods and applications

Most development within electronic structure theory focuses on treating the electronic ground state, but there are a range of standard methods available for describing electronic excited states that involve different tradeoffs between accuracy and computational feasibility. The strengths and weaknesses of some standard electronic structure methods for molecular excited states will be briefly reviewed as a motivation for new work that forms the core of this talk. The goal is to develop electronic structure methods that can correctly treat the ground and excited states of molecules where the electrons exhibit strong electron correlations. Such systems include partially broken bonds, organic diradicaloids and polyradicaloids, antiferromagnetically coupled transition metal centers, etc. We argue that spin-flipping is an ideal approach because there is a well-defined single configuration that serves as a reference for describing the multiconfigurational states where strong correlations are in play. A method that is variational, size-consistent, and applicable to quite large systems is introduced, that we call the restricted active space spin flip (RAS-SF) model. A variety of applications, including the key excited states associated with singlet fission in organic pentacene crystals, as well as a variety of organic polyradicaloids, will be presented to illustrate the capabilities of the method.



Host: Robin Santra - CFEL Theory Division