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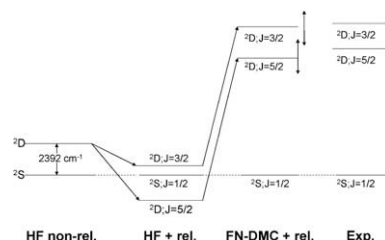
FRONTIERS ARTICLE

1–10

Quantum Monte Carlo for atoms, molecules and solids

William A. Lester Jr., Lubos Mitas, Brian Hammond

The quantum Monte Carlo method for the electronic structure of atoms, molecules, and solids is summarized.



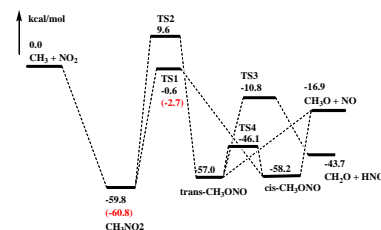
GASEOUS MOLECULES

11–16

CH₃NO₂ decomposition/isomerization mechanism and product branching ratios: An *ab initio* chemical kinetic study

R.S. Zhu, M.C. Lin

Energy diagrams (in kcal/mol) for the CH₃NO₂ decomposition, computed at the UCCSD(T)/CBS level. The values for CH₃NO₂ and TS1 in the parenthesis were calculated at the CASPT3(8,8)/6-311+G(3df,2p)//CASSCF(8,8)/6-311+G(d) level.

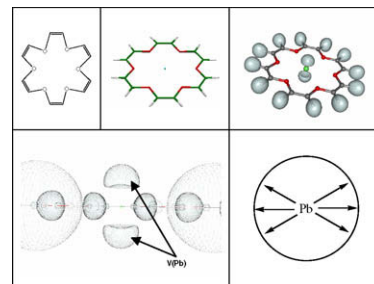


17–19

Beyond holo/hemidirectionality in Pb(II) complexes: Can the valence lone pair be *bisdirected*?

M.-C. van Severen, J.-P. Piquemal, O. Parisel

The possibility of a bisdirectionality of the Pb²⁺ 6s² valence lone pair is for the first time uncovered.

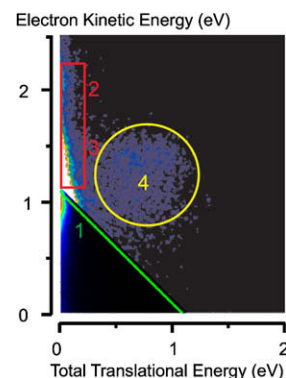


20–27

Revealing femtosecond multiphoton induced multichannel molecular ionization and fragmentation dynamics by photoelectron-photoion coincidence imaging

Arno Vredenburg, Wim G. Roeterdink, Cornelis A. de Lange, Maurice H.M. Janssen

Photoelectron-photoion coincidence imaging unravels four and five photon femtosecond dynamics in ionization and dissociation processes.

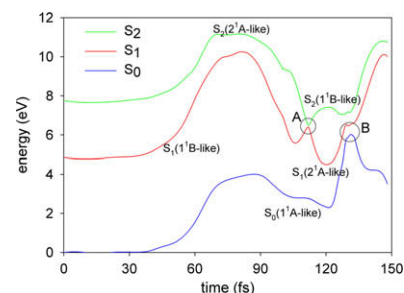


28–32

Semiclassical dynamic simulation of photon induced ring-opening of cyclohexadiene to hexatriene

Anyang Li, Shuai Yuan, Yusheng Dou, Yubin Wang, Zhenyi Wen

The energy curves by CASSCF (6, 6)/MRPT2 calculations for the simulation path. **A**: S_1 - S_2 conical intersection minimum. **B**: S_1 - S_0 non-adiabatic transition.



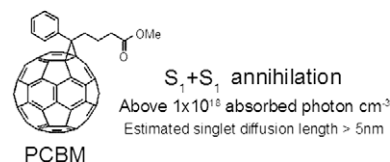
CONDENSED PHASES

33–36

Estimate of singlet diffusion lengths in PCBM films by time-resolved emission studies

Steffan Cook, Akihiro Furube, Ryuzi Katoh, Liyuan Han

Annihilation in PCBM measured by time-resolved emission studies.

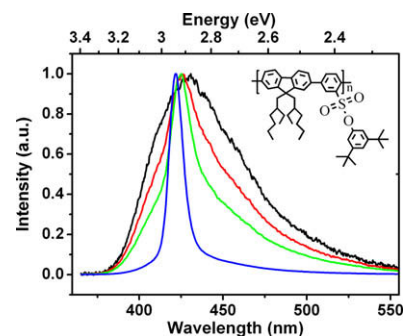


37–41

Amplified spontaneous emission in optically pumped neat films of a polyfluorene derivative

Jiu Yan Li, Frédéric Laquai, Gerhard Wegner

Amplification of deep blue light was observed in the optical waveguide of a novel fluorene-based light-emitting polymer (see picture). The gain property was investigated using the established variable stripe length technique, with the aim to critically elucidate some problems of this experimental method including data treatment and to provide a modification.



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