Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Theoretical studies of the structures and optical properties of the dimers of the fluorene and carbazole derivatives.[1] JOLANTA LAGOWSKI, Memorial University of Newfoundland, ZHIJUN GONG, Yangtze University — The intrinsic properties of the ground and excited states of fluorene, carbazole, fluorene-vinylene and fluorene-acetylene dimers and fluorene-carbazole unit are studied. The ground state optimized structures and energies are obtained using the molecular orbital theory and the density functional theory (DFT). The ground state potential energy curves of the dimers are also obtained. All molecules are nonplanar in their electronic ground states. The character and energy of the first 20 singlet-singlet electronic transitions are investigated by applying the time-dependent DFT approximations to the correspondingly optimized ground state geometries. The lowest singlet state is studied with the configuration interaction (singles) approach (CIS). CIS results suggest geometry relaxation in the first singlet excited state.

[1]This work was supported in part by the Natural Science and Engineering Research Council of Canada. The calculations were performed on ACEnet computational resources.

Jolanta Lagowski
Memorial University of Newfoundland

Date submitted: 23 Nov 2007 Electronic form version 1.4