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Study of Singlet-Triplet Gaps in π-Conjugated Polymers versus Graphene Nanoribbons and Single-Walled Carbon Nanotubes. The Effect of Dimensionality[1] KARAN ARYANPOUR, SUMIT MAZUMDAR, Department of Physics, University of Arizona, HONGBO ZHAO, School of Physics and Telecommunication Engineering, South China Normal University — We compute and compare the gap between the optical singlet and lowest triplet excitons in poly (para-phenylenevinylene) (PPV) with semiconducting graphene nanoribbons (GNRs) and single-walled carbon nanotubes (SWCNTs) within Coulomb correlated model Hamiltonian. The singlet-triplet gaps in semiconducting GNRs and SWCNTs are more than one order of magnitude smaller that in PPV. We ascribe this to two-dimensionality. Spatial distribution of the electron-hole separation in excitons reveals significant localization of the triplet state wave function compared to singlet state in PPV. In GNRs and SWCNTs however, singlet and triplet wave functions exhibit comparably extended spatial distributions. Singlet-triplet gap size is an indicator of the effective Coulomb interaction strength which in turn controls the exciton binding energies of these systems. Exciton binding energy plays a deciding role in light emission and device performance in photovoltaics.

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