Abstract Submitted
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Theoretical Investigation Optical Properties of $Si_{12}C_{12}$ Clusters and Oligomers having Potential as Excitonic Materials[1] XIAOFENG DUAN, Air Force Research Laboratory, AFRL RCM, LARRY BURGGRAF, Air Force Inst of Tech - WPAFB — SiC clusters may have potential in 2-D exciton circuits. We determined the most stable Si_nC_n isomer structures ($n \leq 12$) out of hundreds to thousands isomers using a method combining Stochastic Potential Surface Search and Pseududopotential Plane-Wave Density Functional Theory Car-Parinello Molecular Dynamics simulated annealing (PSPW-CPMD-SA). Four low-energy $Si_{12}C_{12}$ isomer structures are discussed to illustrate the varying optical properties of clusters with structures: i) cage type with C- and Si- segregations, ii) symmetric type formed having π-stacked C aromatic rings and exterior Si regions, iii) nearly planar bowl with C fullerene fragment surrounded by Si atoms, and iv) symmetrical SiC cluster having alternate SiC bonding in the structure. We employed B3LYP and PBE0 functionals and both cc-pVTZ and aug-cc-pVTZ basis sets to perform TDDFT calculations of excitation energies and photo-absorption spectra to show how structure and bonding patterns affect photo excitations in different types of SiC clusters. The electron and the hole charge distribution patterns in excitation were calculated for major photoabsorption transitions, reported for the most stable isomer, closo $Si_{12}C_{12}$. To understand electric field effects we also calculated dynamical polarizabilities for all the four structures using Coupled Perturbed Hartree-Fock (CPHF) at B3LYP/aug-cc-pVTZ and PBE0/aug-cc-pVTZ level of theory.

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