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Exciton Resonances in Novel Silicon Carbide Polymers[1] LARRY BURGGRAF, Air Force Institute of Technology, XIAOFENG DUAN, Air Force Research Laboratory and Air Force Institute of Technology — A revolutionary technology transformation from electronics to excitionics for faster signal processing and computing will be advantaged by coherent exciton transfer at room temperature. The key feature required of exciton components for this technology is efficient and coherent transfer of long-lived excitons. We report theoretical investigations of optical properties of SiC materials having potential for high-temperature excitonics. Using Car-Parinello simulated annealing and DFT we identified low-energy SiC molecular structures. The closo-$Si_{12}C_{12}$ isomer, the most stable 12-12 isomer below 1100 C, has potential to make self-assembled chains and 2-D nanostructures to construct exciton components. Using TDDFT, we calculated the optical properties of the isomer as well as oligomers and 2-D crystal formed from the isomer as the monomer unit. This molecule has large optical oscillator strength in the visible. Its high-energy and low-energy transitions (1.15 eV and 2.56 eV) are nearly pure one-electron silicon-to-carbon transitions, while an intermediate energy transition (1.28 eV) is a nearly pure carbon-to-silicon one-electron charge transfer. These results are useful to describe resonant, coherent transfer of dark excitons in the nanostructures.

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