Exploring the Geometric and Electronic Properties of Palladium Doped Silicon Clusters

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Transition metal-doped silicon clusters have unique properties and have been studied as building blocks for nanomaterials and microelectronics. Here, the structure and properties of candidate palladium doped silicon clusters (Si_nPd_2: n=1-17) were determined using global optimization techniques on a high performance computing cluster at the San Diego Supercomputing Center. Then geometric structures were further optimized utilizing the B3LYP method with 6-311+G(d) basis sets for silicon and lanl2dz pseudopotential for palladium, followed by the larger DSDPBEP86 method with 6-311+G(2d) basis sets for silicon and SDD pseudopotential for palladium, as implemented in the Gaussian 16 program package. The energetics for each cluster size were compared to determine global minima, and the NBO7 program was used to analyze the internal bonding characteristics of each cluster. New lowest energy isomers have been discovered for several sizes investigated. The structures of these newly discovered isomers will be presented noting the transition from exohedral to endohedral doped Pd atoms, the growth pattern in this size range, and the cluster structure versus stability and charge distribution relationships.