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Structural and electronic properties of metal endohedral silicon clusters

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Needless to say, a bulk silicon crystal has the diamond structure, in which each silicon atom has tetrahedral bonds to four neighbors via the sp^3 hybrid orbitals. In contrast, small clusters composed of a few silicon atoms have alternative networks with a denser packing than the diamond structure to terminate the dangling bonds among themselves. Knowing that the silicon bonding networks are changeable depending on various parameters such as the system size and the way the silicon atoms are arranged, it is intriguing to challenge fabricating silicon cage clusters similar to carbon fullerenes. However, it is apparently difficult to make cage structures using silicon atoms because of a strong tendency toward the sp^3 rather than sp^2 hybridization. In 2001, synthesis of silicon cage clusters has been reported. The silicon cage is stabilized when a transition metal atom is enclosed inside the cage due to a strong overlap between the d orbitals of metal and the silicon dangling bonds pointing inward the cluster cavity. It has been predicted a possible form of semiconducting ultra-thin films based on arrangement of the metal endohedral silicon clusters ($M@Si_n$) in two dimensions. In addition, three dimensional assembly of $M@Si_n$ is a promising candidate material to release the Fermi-level pinning at the metal-n-type-Ge interfaces.

Biography

Takehide Miyazaki is the leader of Non-equilibrium Materials Simulation Group in Nanosystem Research Institute of AIST. His major interest is in theoretical modeling of materials with complex structures such as atomic clusters, doped wide band-gap semiconductors and amorphous metal oxides. His study has been cited more than 350 times since its publication by not only research papers but also by review articles and textbooks.

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