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Structure and stability of the $M_{8-n}N_nC_{12}$ (M=Ti, Zr; N=Sc, Y and n=1,2,3) Met-Cars as building blocks of cluster-assembled materials CUNEYT BERKDEMIR, SHI-BO CHENG, A. WELFORD CASTLEMAN JR., Department of Chemistry and Physics, The Pennsylvania State University, JORGE O. SOFO, Depatment of Physics and Materials Research Institute, The Pennsylvania State University — Clusters can be used as building blocks for new materials. However, in order to form a bulk material with clusters, they should be chemically stable. This stability can be characterized by a closed-shell electronic configuration having a large HOMO-LUMO gap. Met-Cars, metal-carbon species composed of early transition metals bonded to carbon, are stable but very reactive. We propose a method to lower their reactivity by metal atom substitution with lower atomic number atoms. We report DFT results on $M_{8-n}N_nC_{12}$ (M = Ti, Zr; N = Sc, Y, and n=1,2,3) Met-Cars in the neutral, cationic and anionic charge states. Our results show that the isoelectronic $M_6N_2C_{12}$, $M_5N_3C_{12}^-$ and $M_7N_1C_{12}^+$ Met-Cars have closed-shell electronic configurations and larger HOMO-LUMO gaps (1.0-1.7 eV) than that of the M_8C_{12}. The inter-cluster interaction between two isolated neutral $M_6N_2C_{12}$ Met-Cars is relatively weak compared to the M_8C_{12} dimers. Due to the weak interaction of the isolated neutral Met-Cars, their unique properties would be retained during assembly.

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