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On Diamond Nucleation Sites and Relativistic Rehybridization in Pyramidalizing Reactions. Boris Udovic, Sezanska 11, 6210 Sezana, Slovenia, boris.udovic@email.si

The experienced low tendency toward carburization reactions and carbon solubility make rather outstanding the chemical behaviour of non-transition elements as metal Sn and Pb atoms among the potential combinations of some most celebrated $3d \rightarrow 6d$ carbide formers in diamond phase synthesis. In the lower valence state a stable but sterically active $6s^2$ electron pair is projected out one side of the Pb atom, generating an asymmetric structure upon filling one of the hybrid orbitals originated from their $6s$ and $6p$ atomic components. The relativistic contraction of the $6s$ orbital and the expansion of the full filled $5d$ kernel envelope promote the reshape of the nearest bonding orbitals. In a possible alloy of more noble metals and non-transition elements as Pb, which are combined with a carbide-former of the iron group (Fe, Th, etc.), the last elements react as carbon attractors while the non-transition element Pb behaves as a repeller-expeller of dissolved carbon atoms. The antagonistic expelling action is expected to involve at least one single bond between surface Pb and carbon ad-atoms. The interacting field turns into the change of the symmetry of the potential energy of surface Pb atoms, which is further desymmetrized and its wavefunction is changed to rehybridize forming the sterically active $6s^2$ lone pair in pyramidal electronic redistribution. The repelling Pauli fields torque the vicinal p_z carbon orbital and gain to release more paraffinic than olefinic bonds in comparison to stronger attractive interactions with carbide and graphite-former elements.