Doped deltahedral organo-Zintl superalkali cations

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Abstract
The doped deltahedral Zintl clusters are known for decades. Here, we report a functionalized doped organo-Zintl clusters $[Ge_7P_2R_3]$(R = CH_3, C_2H_5 & C_3H_3) derived from the doped $[Ge_7P_2]^{2-}$ Zintl ion by replacing germanium atoms in deltahedral Ge_9^{4-} cluster with Phosphorus (P). Using first principle calculation, we show that, it is also possible to design superalkali compounds by using doped deltahedral Zintl ions as a core with suitable organic aliphatic and cyclic ligands. The calculated vertical electron affinities (VEAs) of designed Zintl complexes are lower than alkali metals ionization energy (IE = 3.89–5.34 eV).

Author keywords
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