Spontaneous formation and stability of small GaP fullerenes

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We report the spontaneous formation of a GaP fullerene cage in ab-initio Molecular Dynamics simulations starting from a bulk fragment. A systematic study of the geometric and electronic properties of neutral and ionized GaP clusters suggests the stability of hetero-fullerenes formed by a compound with zincblend bulk structure. We find that GaP fullerenes up to 28 atoms have high symmetry, closed electronic shells, large HOMO-LUMO energy gaps and do not dissociate when ionized. We compare our results for GaP with those obtained by other groups for the corresponding BN clusters.