Supplementary Information: Theoretical Method

We have used Density Functional Theory (DFT) under the Local Density Approximation (LDA) as implemented in the AIMPRO package.[22] The calculations were carried out using supercells, fitting the charge density to plane waves within an energy cut-off of 225 Ry. Charge density oscillations in partly-filled degenerate orbitals during the self-consistency cycle were damped using a Fermi occupation function with kT=0.04 eV. Atom-centered Gaussian basis functions are used to construct the many-electron wave function. These functions are labelled by multiple orbital symbols, where for each symbol the Gaussians are multiplied by spherical harmonics including all angular momenta up to maxima *p* (l=0,1) and *d* (l=0,1,2), respectively. Following this nomenclature, the basis sets used for each atom type were *pdddp* (P), *dddd* (N), *ddpp* (O), and *ppp* (H). Carbon atoms used a contracted sum basis set equivalent of *C44G**. A Bloch sum of these functions is performed over the lattice vectors to satisfy the periodic boundary conditions of the supercell. Calculation were performed on a large hexagonal unit cell (a=14.28Å, c=12.29Å), with Brillouin zone sampling 1x1x1 k-points within the Monkhorst-Pack scheme. Radical calculations were performed spin polarised. Atomic positions were optimised using a conjugate gradient scheme. In the analysis, standard states for carbon, nitrogen and phosphorus when calculating exothermicities were taken as C_{60}, N_2 and P_4 respectively.