Supplementary Information for

# Why is $BeGeN_2$ different? A computational bonding analysis

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## 1) Computational details

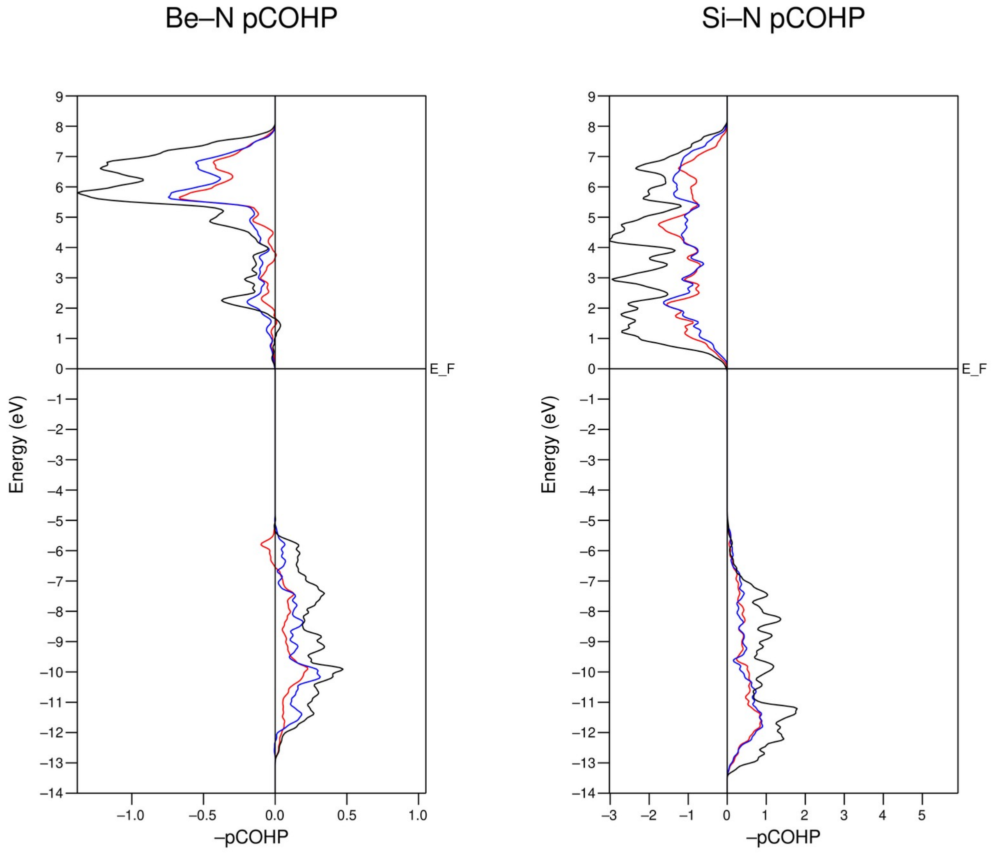
The crystal structures of all compounds within the study were first geometrically optimised using the BFGS algorithm implemented in Quantum Espresso. Structures were optimised using the respective space group symmetry, and with convergence criteria on energy ($< 10^{-6}$ Ry), force ($< 10^{-4}$ Ry/Bohr) and cell pressure ($< 10^{-2}$ kbar).
SCF calculations as LOBSTER input were then prepared using time reversal symmetry only.
All calculations were uniformly performed using PBEsol exchange-correlation potential PAW pseudopotentials with uniform kinetic energy cutoff (70 Ry) and charge density cutoff (700 Ry). All calculations were performed using a 12 x 12 x 12 Monkhorst-Pack k-point grid.

LOBSTER calculations were performed in a range of -35 eV to +15 eV in order to sample all valence electrons within the partition. Fits were done to the pbeVaspFit2015 basis set using the recommended basis functions as automatically selected by Lobster. *M*-*M* bonds up to 4 Å were considered for the calculation of the next nearest neighbour interactions.

## 2) COHP Plots

The colour choices are the same as in the main text figure 3

$BeSiN_2$ – *Pmc*$2_1$



MgGeN$_2$ – $Pmc2_1$