Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

We performed a convergence test to examine the effect of the k-points grid density on the calculated formation enthalpies H_{CP}. In VASP, the KSPACING parameter is responsible for the density of k-points. The value of 0.1 corresponds to the high k-point density; the value of 0.5 corresponds to the low k-point density.

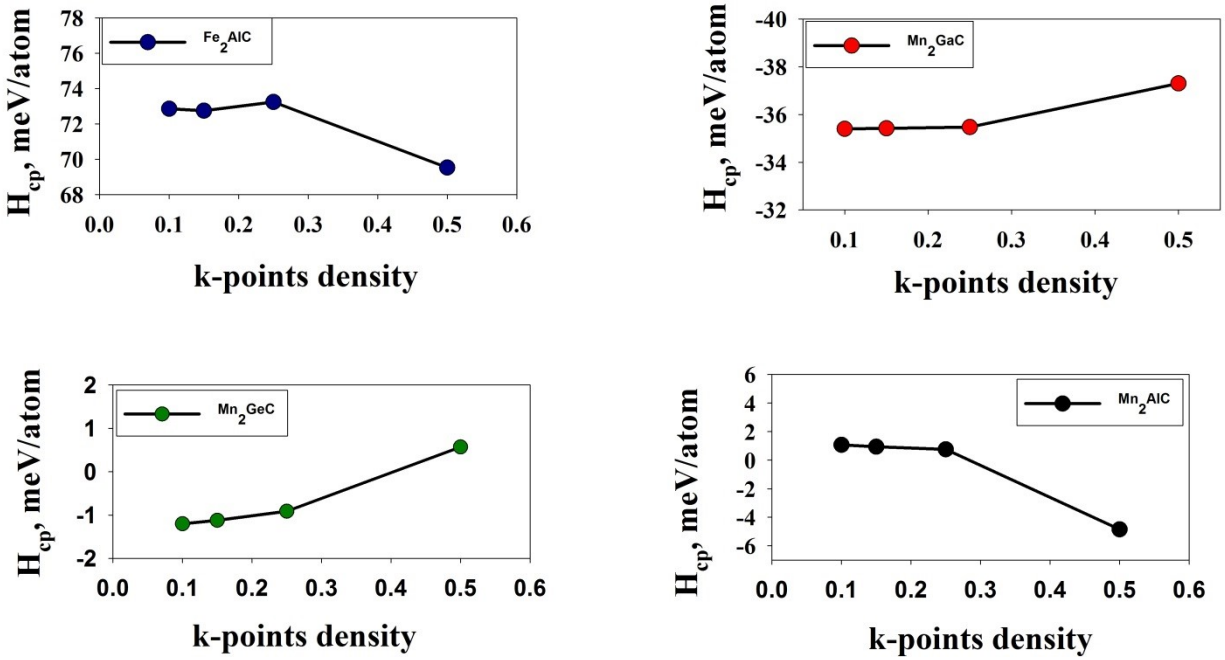

Figure S1. Formation enthalpy H_{CP} as function of k-point density. 0.1 corresponds to the high k-point density, 0.5 corresponds to the low k-point density

As one can see from Figure S1, an increase in the density of k-points leads to convergence of the results when the KSPACING parameter is higher than 0.2. Therefore, through all calculations, we used KSPACING = 0.15.