

Structural and magnetic properties of NiC_x and NiN_x (x = 0 to 1/3) solid solutions from first-principles calculations

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Table S1. Calculated dimensions of the calculation supercells for dilute C/N atoms in fcc and hcp lattices with C/N atoms at octahedral sites. The corresponding structures are displayed in Fig. S1.

figure	Composition	lattice/stacking	Parameters (Å)
S-1c)	Ni ₃₂ C	fcc/	$a = 7.097$
S-1c)	Ni ₃₂ N	fcc/	$a = 7.489$
S-1a)	Ni ₅₄ C	hex_fcc/abcabc	$a = 7.505$ $c = 12.261$
S-1a)	Ni ₅₄ N	hex_fcc/abcabc	$a = 7.506$ $c = 12.261$
S-1b)	Ni ₅₄ C	hcp/ababab	$a = 7.489$ $c = 12.346$
S-1b)	Ni ₅₄ N	hcp/ababab	$a = 7.489$ $c = 12.346$
S-1f)	Ni ₃₂ C ₂	Fcc (C far away from each other)	$a = 7.142$

Table S2. Calculated local electronic configurations (EC, electrons), local magnetic configuration (MC, μ_B), and total magnetic moments (M, μ_B) at the Ni sites as nearest neighbors (NN, shell_1), and the next nearest neighbors (NNN, shell_2). The results for pure fcc-Ni metal are included for the sake of comparison.

Ni sites	Ni ₃₂ C	Ni ₃₂ N
Shell_1	EC: $4s^{0.565} 4p^{0.685} 3d^{8.534}$	EC: $4s^{0.549} 4p^{0.669} 3d^{8.513}$
X-6Ni	MC: $4s^{-0.01} 4p^{-0.02} 3d^{0.25}$ Moment: 0.23	MC: $4s^{-0.01} 4p^{-0.02} 3d^{0.24}$ Moment: 0.22
Shell_2	EC: $4s^{0.552} 4p^{0.584} 3d^{8.468}$	EC: $4s^{0.552} 4p^{0.582} 3d^{8.468}$
X-8Ni	MC: $4s^{-0.01} 4p^{-0.02} 3d^{0.64}$ M: 0.61	MC: $4s^{-0.01} 4p^{-0.02} 3d^{0.66}$ M: 0.63
pure fcc-Ni	EC: $4s^{0.566} 4p^{0.609} 3d^{8.464}$ MC: $4s^{-0.01} 4p^{-0.03} 3d^{0.67}$ Moment: 0.63	

Supplementary Figure S1 (a-i): Schematics of supercells used for different NiX_y ($X = \text{C/N}$) phases. The blue spheres represent Ni atoms, the green spheres C/N atoms.

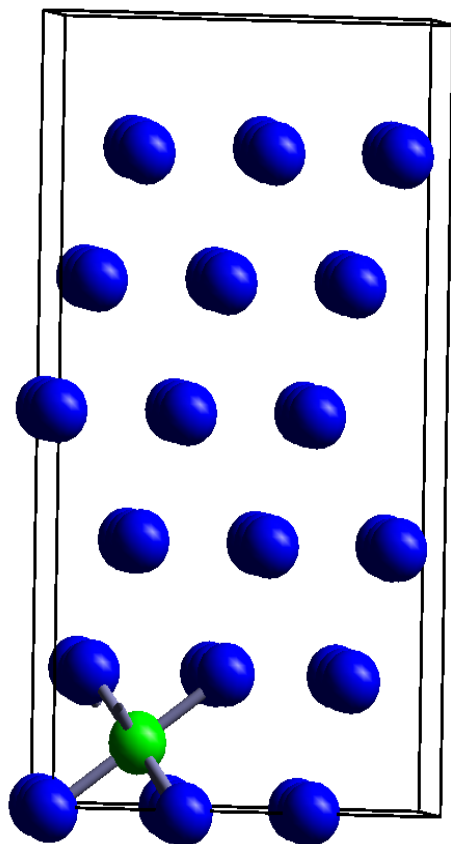


Figure S1a: hex_fcc/abcabc_Ni₅₄X

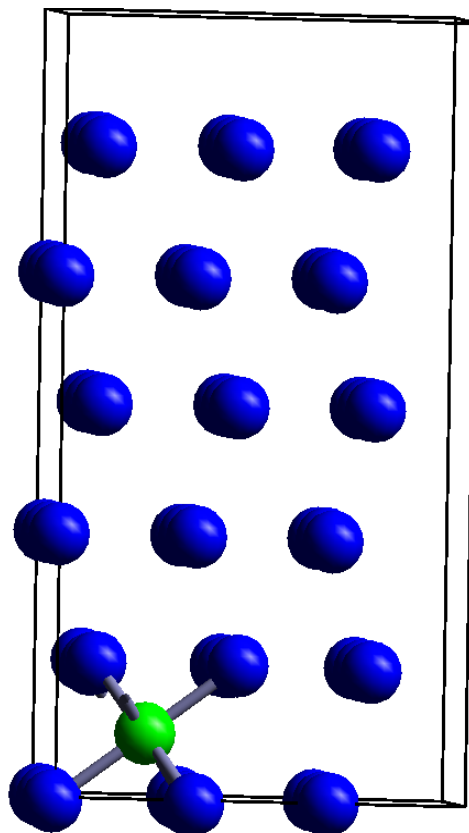


Figure S1b: hcp/ababab_Ni₅₄X

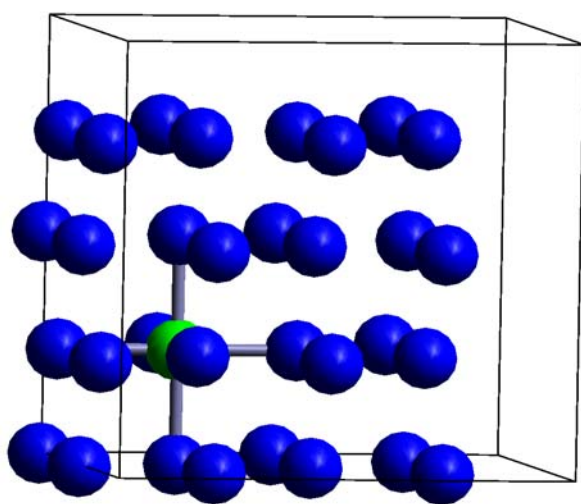


Figure S1c: fcc-Ni₃₂X_{oct}

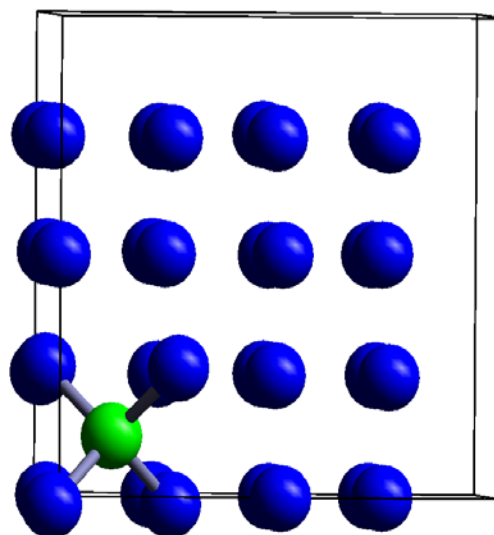


Figure S1d: fcc-Ni₂X_{tetra}

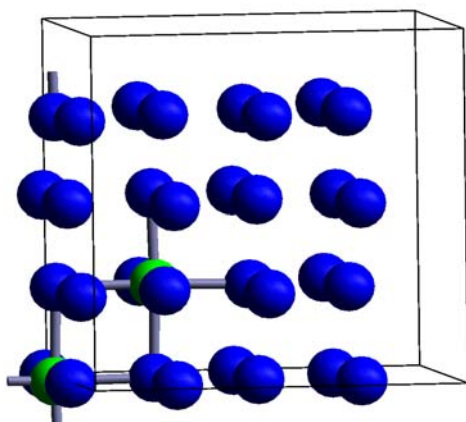


Figure S1e: fcc-Ni₃₂X₂_close

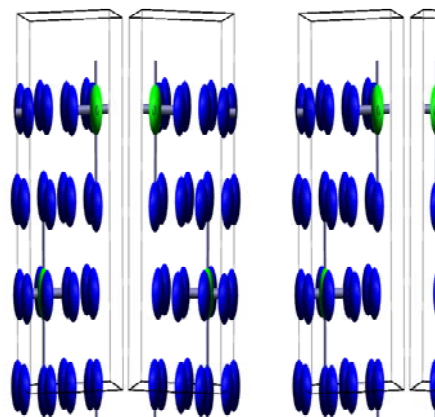


Figure S1f: fcc-Ni₃₂X₂_far

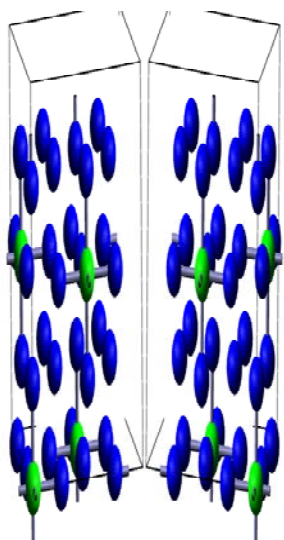


Figure S1g: fcc-Ni₃₂X₄ (Ni₈X)

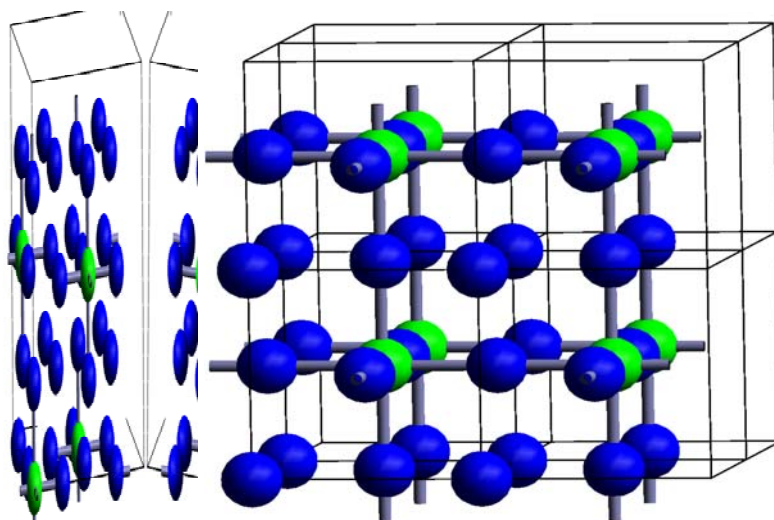


Figure S1h: fcc-Ni₃₂X₈ (Ni₄X)

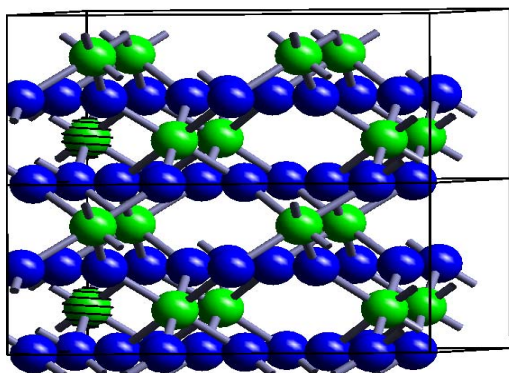


Figure S1i: hcp-Ni₂₄X₉, Striped green indicates C atoms at b sites