Structure, stability, electronic and magnetic properties of Ni$_4$ clusters containing impurity atoms

Petko St. Petkov,[1] Georgi N. Vayssilov,[1]* Sven Krüger,[2] and Notker Rösch[2]*

[1] *Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria,*
    e-mail: gnv@chem.uni-sofia.bg

[2] *Department Chemie, Technische Universität München, 85747 Garching, Germany,*
    e-mail: roesch@ch.tum.de

ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. BE of impurity atoms in symmetric positions on a Ni$_4$ cluster. Structures in bold are reported in the text, while the other structures do not correspond to local minima. For notation of the structures see Fig. S1.

Complex	BE (kJ/mol)		
	H	O	C
(μ_4-X)Ni$_4$/T$_d$	76	198	516
(?-X)Ni$_4$/C$_{3v}$	207	320	363
(μ_4-X)Ni$_4$/C$_{3v}$	98	324	593
(μ_3-X)Ni$_4$/C$_{3v}$	250	430	**629**
(μ_4-X)Ni$_4$/C$_{2v}$	-	359	**640**
(μ-X)Ni$_4$/C$_{2v}$	**286**	**455**	-
(μ_4-X)Ni$_4$/D$_{4h}$	161	267	610
(μ_4-X)Ni$_4$/C$_{4v}$	161	279	610
(μ_4-X)Ni$_4$/C$_{2v}$-pl	-	383	**628**

a) $(\mu_4\text{-X})Ni_4/T_d$

b) $(\eta\text{-X})Ni_4/C_{3v}$

c) $(\mu_4\text{-X})Ni_4/C_{3v}$

d) $(\mu_3\text{-X})Ni_4/C_{3v}$

e) $(\mu_4\text{-X})Ni_4/C_{2v}$

f) $(\mu\text{-X})Ni_4/C_{2v}$

g) $(\mu_4\text{-X})Ni_4/D_{4h}$

h) $(\mu_4\text{-X})Ni_4/C_{4v}$
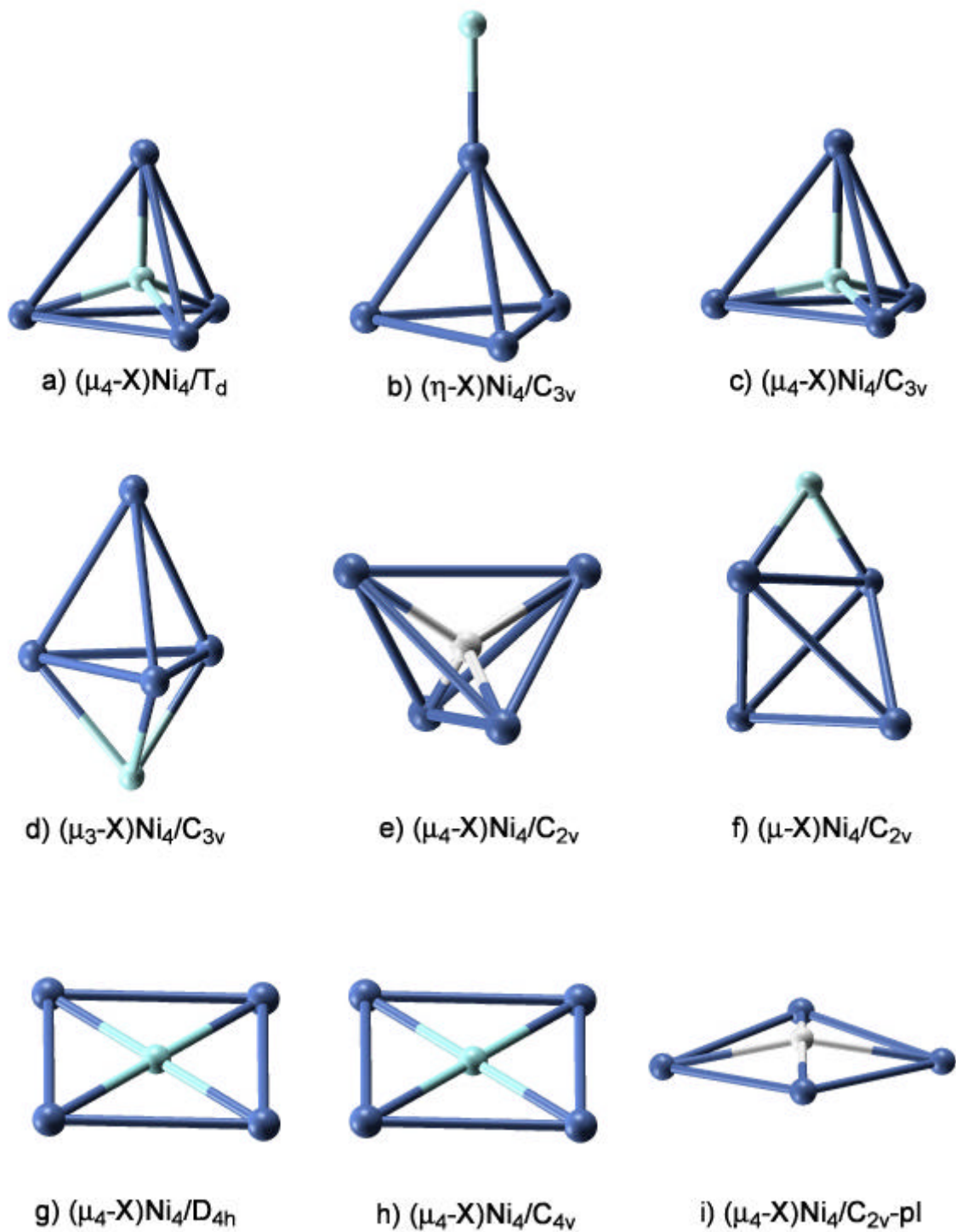
i) $(\mu_4\text{-X})Ni_4/C_{2v}\text{-pl}$

Figure S1
Initial structures for search of the location of the impurity atoms on the clusters.
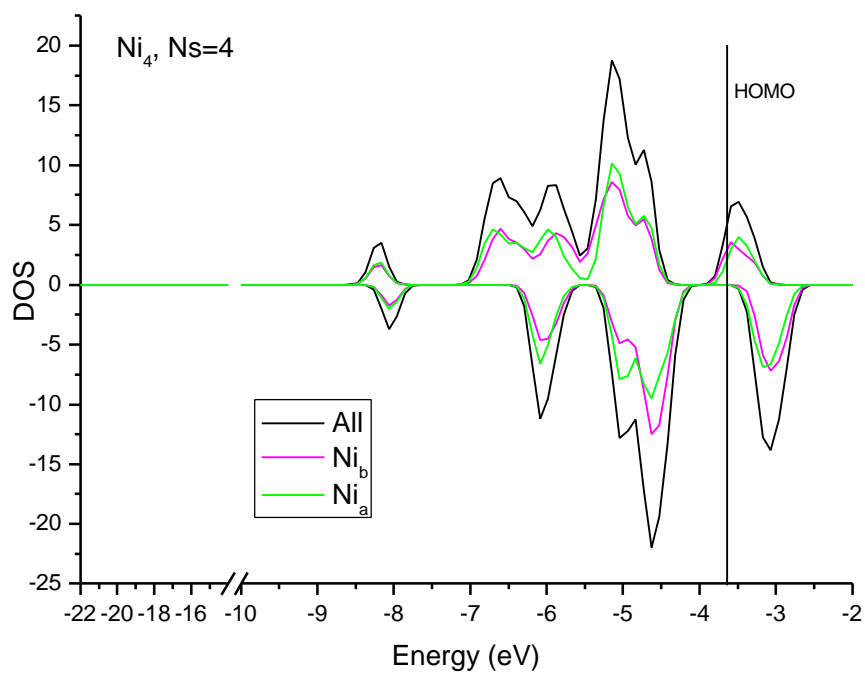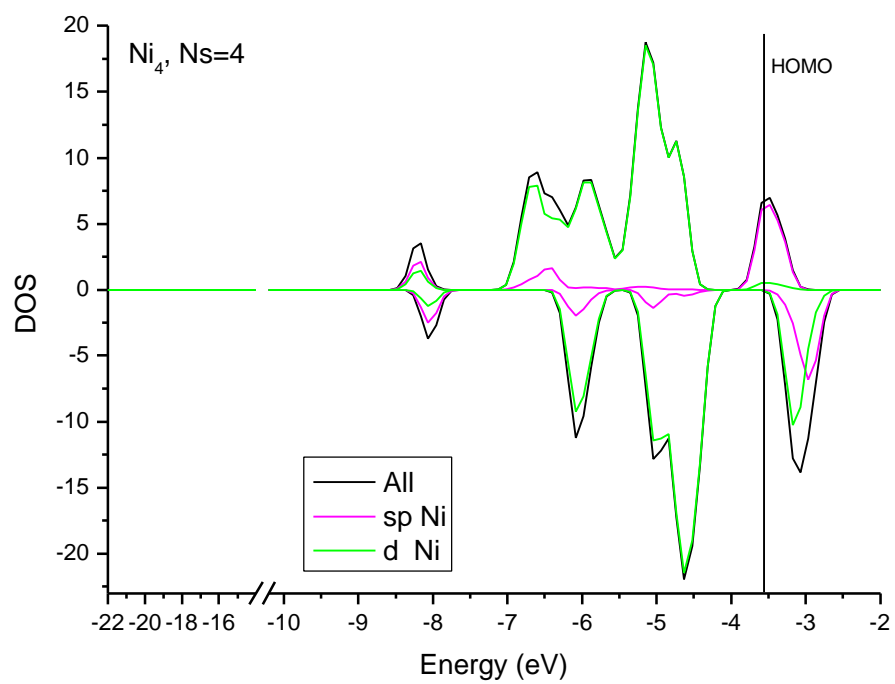
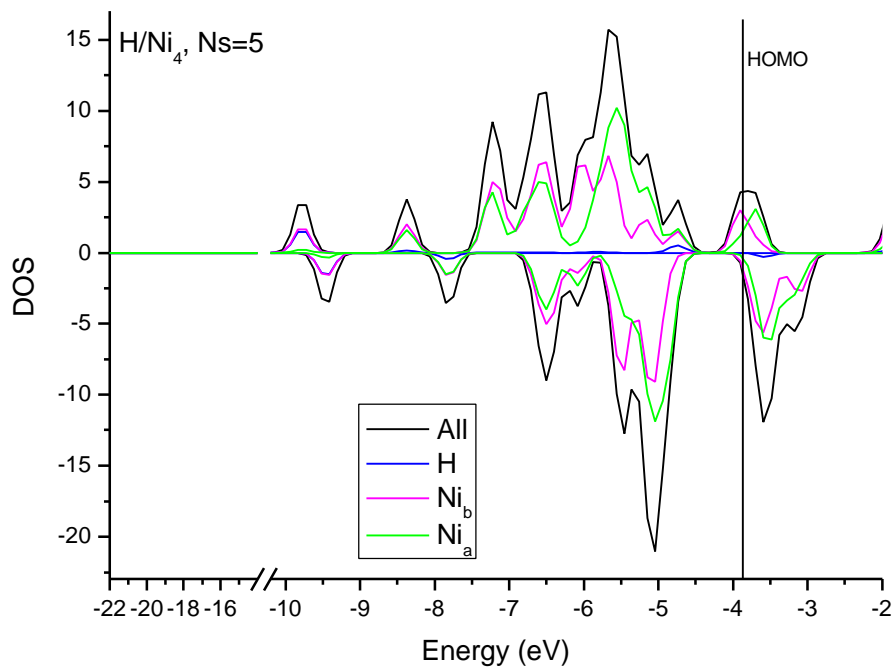**Figure S2**
Density of states (DOS) for bare Ni$_4$/C$_{2v}$
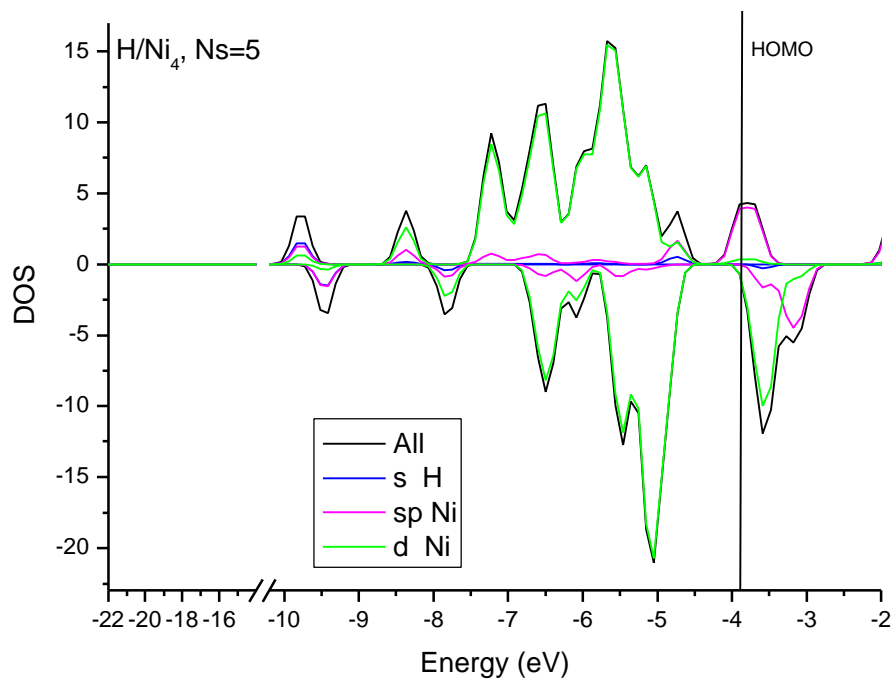
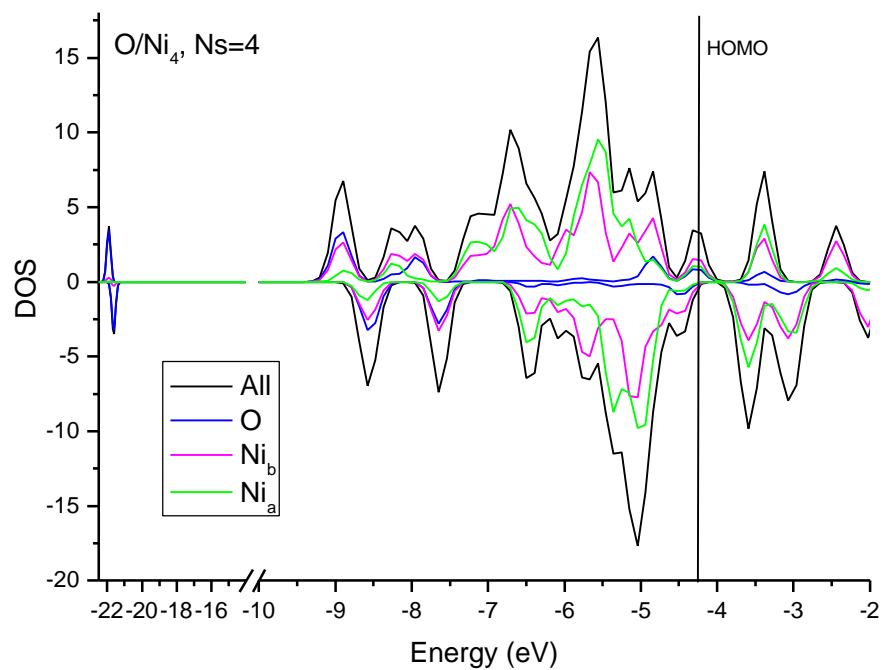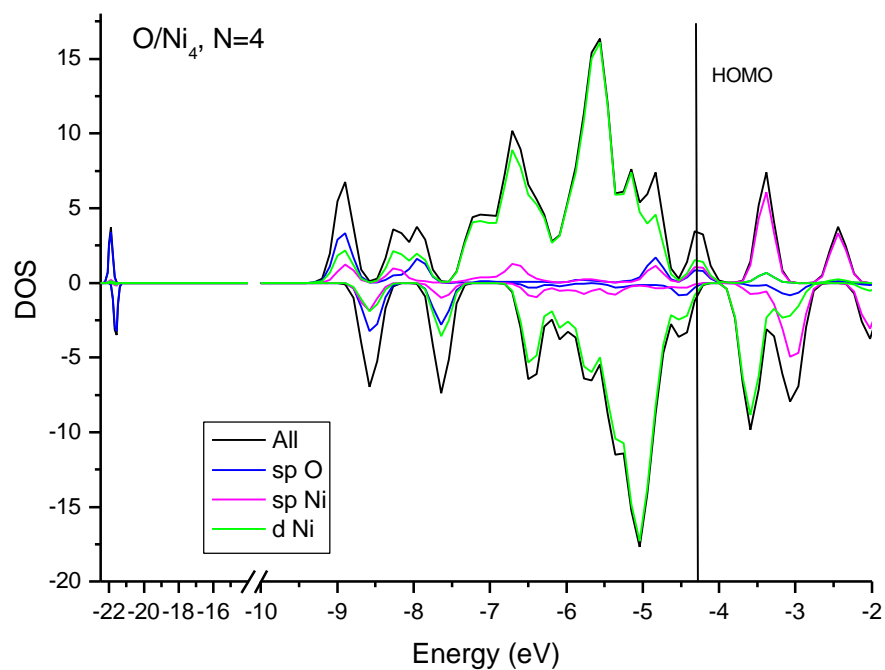**Figure S3**

Density of states (DOS) for (μ-H)Ni$_4$/C$_{2v}$(5).

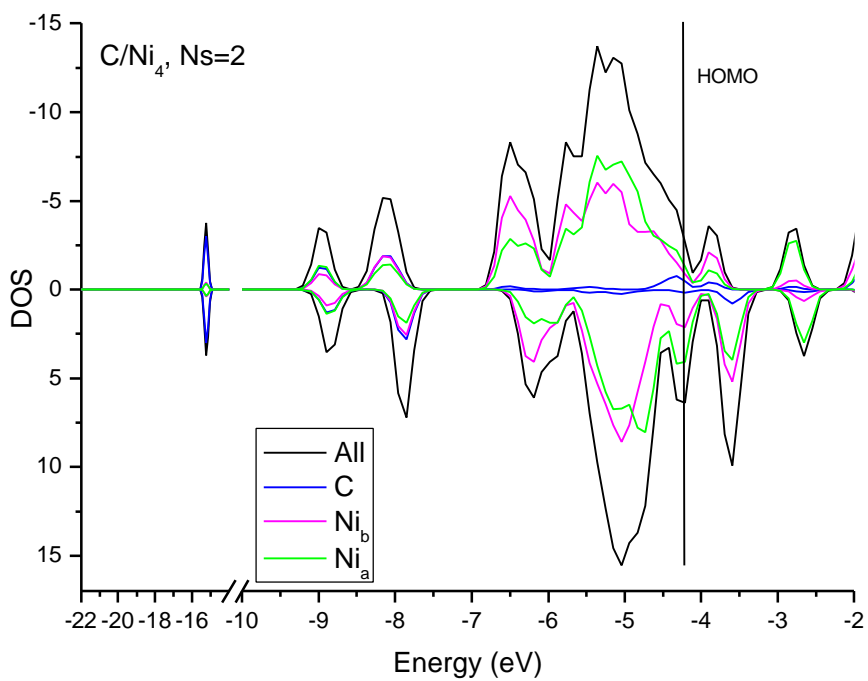**Figure S4**
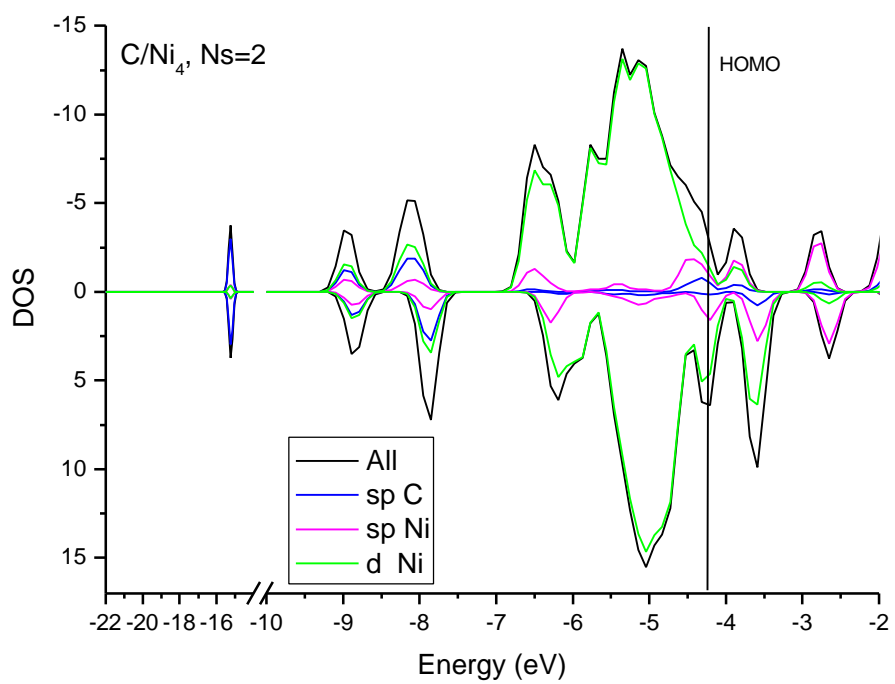
Density of states (DOS) for $(\mu\text{-O})Ni_4/C_{2v}$.

Figure S5
Density of states (DOS) for (μ_4-C)Ni$_4$/C$_{2v}$.