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Photoelectron velocity-map imaging spectroscopy of nickel carbide: Examination of the low-lying electronic states

Zhiling Liu,*, [1] Qingyang Lin,[1] Ya Li,[1] Jing He,[1] Jingmei Jiao,[1] Lianxia Liu,[1] Yonghong Yan,[1] Hai-Shun Wu,[1] Fuqiang Zhang,[1] Jianfeng Jia,[1] and Hua Xie*, [2]

[1]*School of Chemical and Material Science, Key Laboratory of Magnetic Molecules & Magnetic Information Materials, the Ministry of Education, Shanxi Normal University. No. 339, Taiyu Road, Taiyuan, Shanxi 030031, China.*

Electronic mail: lzling@sxnu.edu.cn.

[2]*State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 457 Zhongshan Road, Dalian, Liaoning 116023, China.*

Electronic mail: xiehua@dicp.ac.cn.

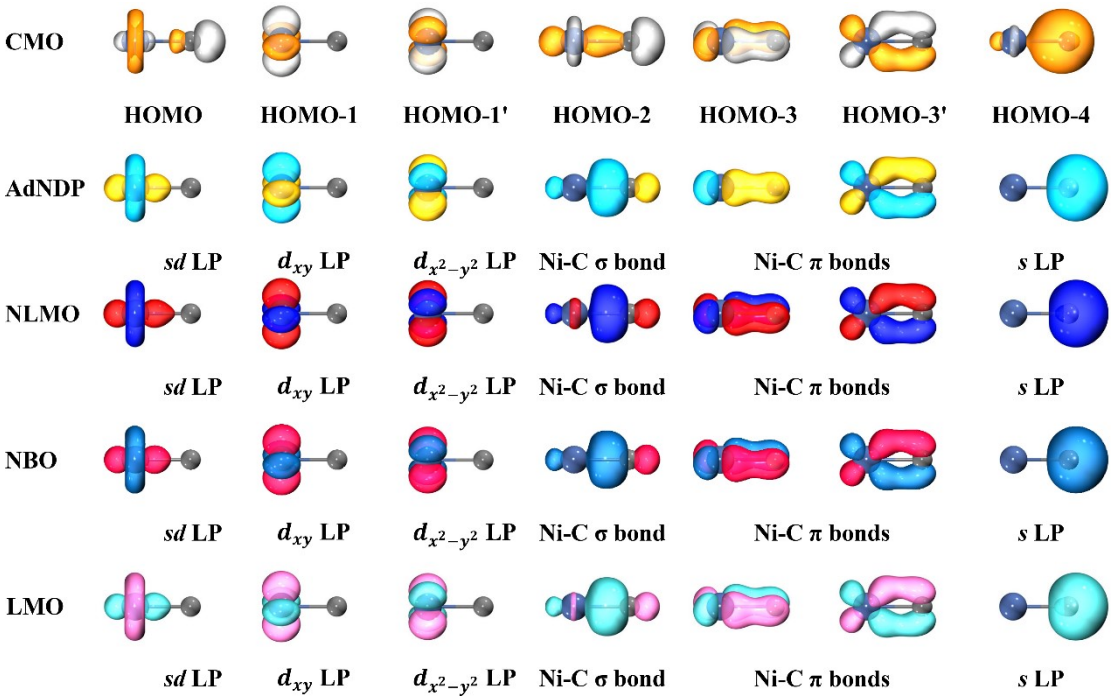

FIG. S1. A comparison of selected CMOs, AdNDP, NLMO, NBO, LMO for the NiC molecule calculated at the BP86-D3(BJ)/def2-TZVPP level. (isosurface = 0.1 au)

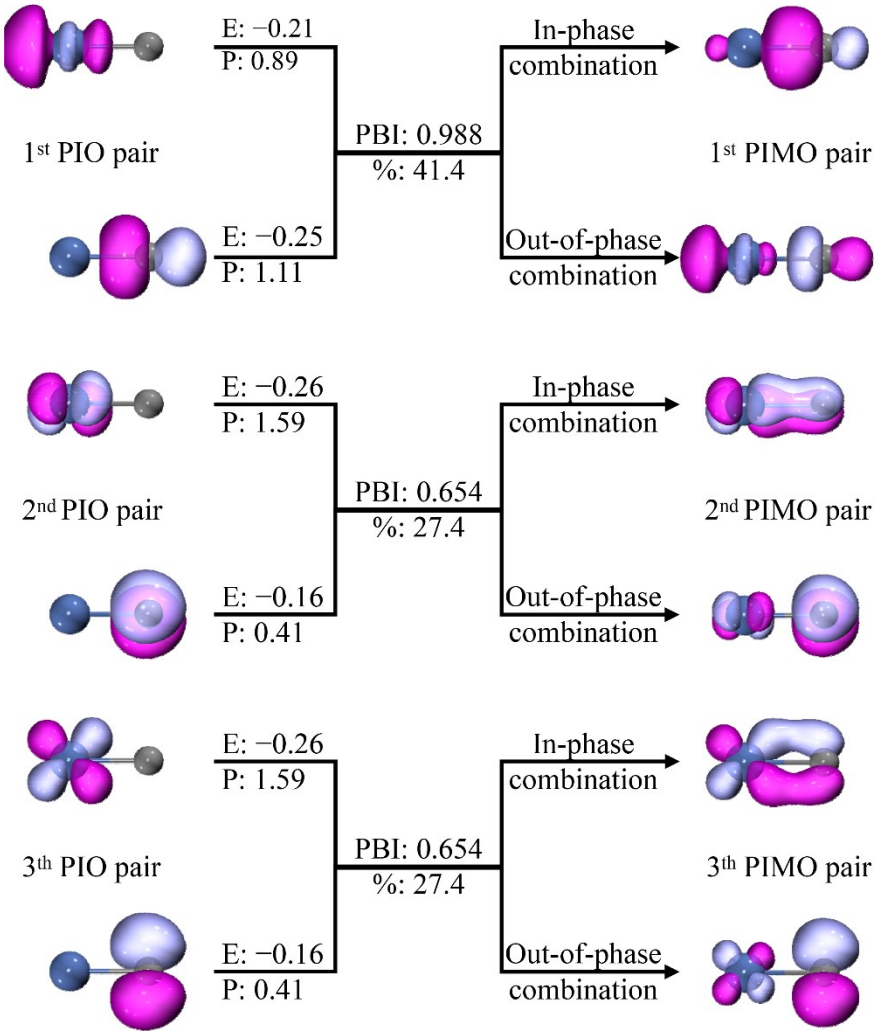

FIG. S2. Results of PIO analysis on NiC with Ni atom and C atom as two fragments at the BP86-D3(BJ)/def2-TZVPP level. (isosurface = 0.1 au)

TABLE S1. EDA-NOCV results for NiC at the BP86-D3(BJ)/TZ2P level using charged nickel ion and carbon ion in different electronic reference configuration as interacting moieties. Energy values are given in kcal·mol^{-1}.

Fragments	C^+ [***D***, $(2s_\sigma)^2(2p_\pi)^0(2p_\sigma)^1$] Ni^- [***D***, $(3d_\pi)^4(3d_\sigma)^2(3d_\delta)^4(4s_\sigma)^1$]	C^- [***Q***, $(2s_\sigma)^2(2p_\pi)^2(2p_\sigma)^1$] Ni^+ [***Q***, $(3d_\pi)^2(3d_\sigma)^2(3d_\delta)^4(4s_\sigma)^1$]	C^- [***D***, $(2s_\sigma)^2(2p_\pi)^3(2p_\sigma)^0$] Ni^+ [***D***, $(3d_\pi)^1(3d_\sigma)^2(3d_\delta)^4(4s_\sigma)^2$]	C^- [***D***, $(2s_\sigma)^2(2p_\pi)^1(2p_\sigma)^2$] Ni^+ [***D***, $(3d_\pi)^3(3d_\sigma)^2(3d_\delta)^4(4s_\sigma)^0$]
Symmetry	$C_{\infty v}$	$C_{\infty v}$	C_{2v}	C_{2v}
ΔE_{int}	−432.12	−303.90	−559.88	−414.52
ΔE_{pauli}	271.92	331.01	236.59	324.86
ΔE_{disp}[a]	−1.19 (0.17%)	−1.19 (0.19%)	−1.19 (0.15%)	−1.19 (0.16%)
ΔE_{elstat}[a]	−311.89 (43.30%)	−391.47 (61.66%)	−230.74 (28.97%)	−393.66 (53.24%)
ΔE_{orb}[a]	−390.95 (55.53%)	−242.25 (38.16%)	−564.54 (70.88%)	−344.54 (46.60%)
$\Delta E_{orb(\sigma)}$[b]	−129.30 (33.07%)	−64.61 (26.67%)	−344.50 (61.02%)	−69.18 (20.08%)
$\Delta E_{orb(\pi)}$[b]	−120.75 (30.89%)	−80.12 (33.07%)	−100.15 (17.74%)	−234.46 (68.05%)
$\Delta E_{orb(\pi')}$[b]	−120.75 (30.89%)	−80.12 (33.07%)	−119.65 (21.19%)	−23.92 (6.94%)

[a]The italic capital letters *D* and *Q* in square brackets stand for the electronic doublet and quartet states, respectively.

[b]The value in parentheses gives the percentage contribution to the total attractive interactions $\Delta E_{disp} + \Delta E_{elstat} + \Delta E_{orb}$.

[c]The value in parentheses gives the percentage contribution to the total orbital interactions ΔE_{orb}.