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Electronic Supplementary Information

A Local Point of View of the Cu(100) → NiTPP Charge Transfer at the NiTPP/Cu(100) interface.

Silvia Carlotto, Alberto Verdini, Giovanni Zamborlini, Iulia Cojocariu, Vitaliy Feyer, Luca Floreano, Maurizio Casarin.

Table S1. Optimized Cartesian Coordinates (Å) of the free D_{4h} Ni(II) tetraphenyl-porphyrin

Atom.	X	Y	Z
Ni	0.0000	0.0000	0.0000
N	0.0000	1.9795	0.0000
N	0.0000	-1.9795	0.0000
N	1.9795	0.0000	0.0000
N	-1.9795	0.0000	0.0000
C	1.0982	2.8212	0.0000
C	-1.0982	2.8212	0.0000
C	1.0982	-2.8212	0.0000
C	-1.0982	-2.8212	0.0000
C	2.8212	1.0982	0.0000
C	2.8212	-1.0982	0.0000
C	-2.8212	1.0982	0.0000
C	-2.8212	-1.0982	0.0000
C	2.4329	2.4329	0.0000
C	2.4329	-2.4329	0.0000
C	-2.4329	2.4329	0.0000
C	-2.4329	-2.4329	0.0000
C	0.6801	4.2039	0.0000
C	0.6801	-4.2039	0.0000
C	-0.6801	4.2039	0.0000
C	-0.6801	-4.2039	0.0000
C	4.2039	0.6801	0.0000
C	4.2039	-0.6801	0.0000
C	-4.2039	0.6801	0.0000
C	-4.2039	-0.6801	0.0000
C	3.4943	3.4943	0.0000
C	-3.4943	3.4943	0.0000
C	3.4943	-3.4943	0.0000
C	-3.4943	-3.4943	0.0000
C	3.9966	3.9966	1.2075
C	3.9966	3.9966	-1.2075
C	3.9966	-3.9966	1.2075
C	3.9966	-3.9966	-1.2075
C	-3.9966	3.9966	1.2075
C	-3.9966	3.9966	-1.2075

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C	-3.9966	-3.9966	1.2075
C	-3.9966	-3.9966	-1.2075
C	4.9847	4.9847	1.2086
C	4.9847	4.9847	-1.2086
C	4.9847	-4.9847	1.2086
C	4.9847	-4.9847	-1.2086
C	-4.9847	4.9847	1.2086
C	-4.9847	4.9847	-1.2086
C	-4.9847	-4.9847	1.2086
C	-4.9847	-4.9847	-1.2086
C	5.4809	5.4809	0.0000
C	-5.4809	5.4809	0.0000
C	5.4809	-5.4809	0.0000
C	-5.4809	-5.4809	0.0000
H	1.3525	5.0494	0.0000
H	-1.3525	5.0494	0.0000
H	1.3525	-5.0494	0.0000
H	-1.3525	-5.0494	0.0000
H	5.0494	1.3525	0.0000
H	-5.0494	1.3525	0.0000
H	5.0494	-1.3525	0.0000
H	-5.0494	-1.3525	0.0000
H	3.6092	3.6092	2.1450
H	3.6092	3.6092	-2.1450
H	3.6092	-3.6092	2.1450
H	3.6092	-3.6092	-2.1450
H	-3.6092	3.6092	2.1450
H	-3.6092	3.6092	-2.1450
H	-3.6092	-3.6092	2.1450
H	-3.6092	-3.6092	-2.1450
H	5.3658	5.3658	2.1514
H	5.3658	5.3658	-2.1514
H	5.3658	-5.3658	2.1514
H	5.3658	-5.3658	-2.1514
H	-5.3658	5.3658	2.1514
H	-5.3658	5.3658	-2.1514
H	-5.3658	-5.3658	2.1514
H	-5.3658	-5.3658	-2.1514
H	6.2487	6.2487	0.0000
H	-6.2487	6.2487	0.0000
H	6.2487	-6.2487	0.0000
H	-6.2487	-6.2487	0.0000

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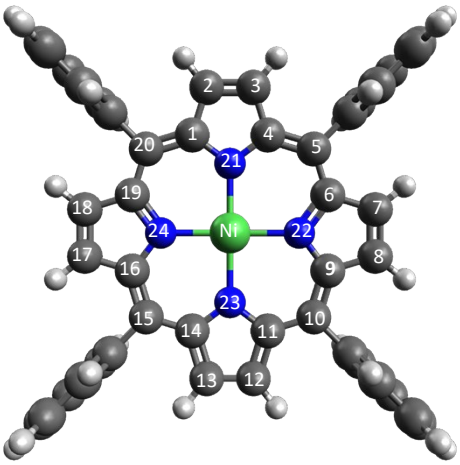

Figure 1. Schematic representation of the D_{4h} NiTPP molecule with the atom numbering recommended by IUPAC for the pristine macrocycle (^{pmc}NiP). White, grey, blue, and green spheres correspond to H, C, N, and Ni atoms. The molecular plane (σ_h) corresponds to the xy one in the adopted framework. Carbon atoms C5, C10, C15, and C20 are collectively labelled meso carbon atoms (C^m). No numbering is provided for carbon atoms of the phenyl groups (collectively labelled C^{Ph}) bonded to C^m.

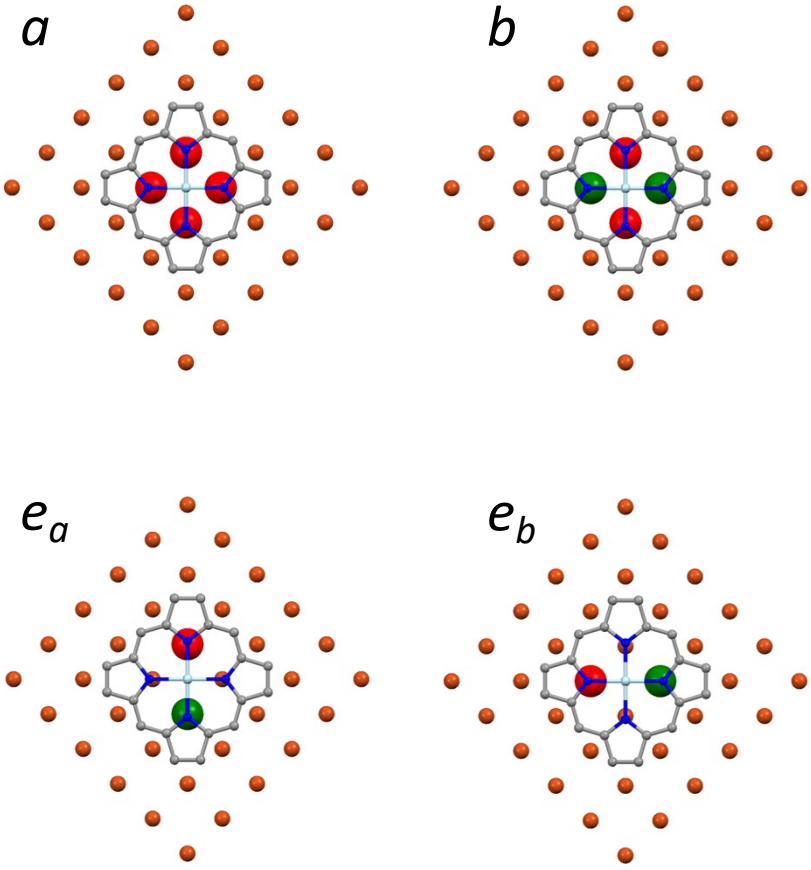

Figure S2. Schematic representation of the ${}^{nn}Cu^{S}_{ffh}$ 4s AOs SALC of symmetry *a*, *b* and *e*. Large red and green spheres represent Cu^S 4s AOs and corresponding different phases. The ^{pmc}NiP planar core of the optimized D_{4h} NiTPP with the Ni–N bonds aligned with the <001> directions and the Ni species at 1.93 Å from the substrate and positioned at the *ffh* site has been superimposed to the substrate in each panel of the figure.

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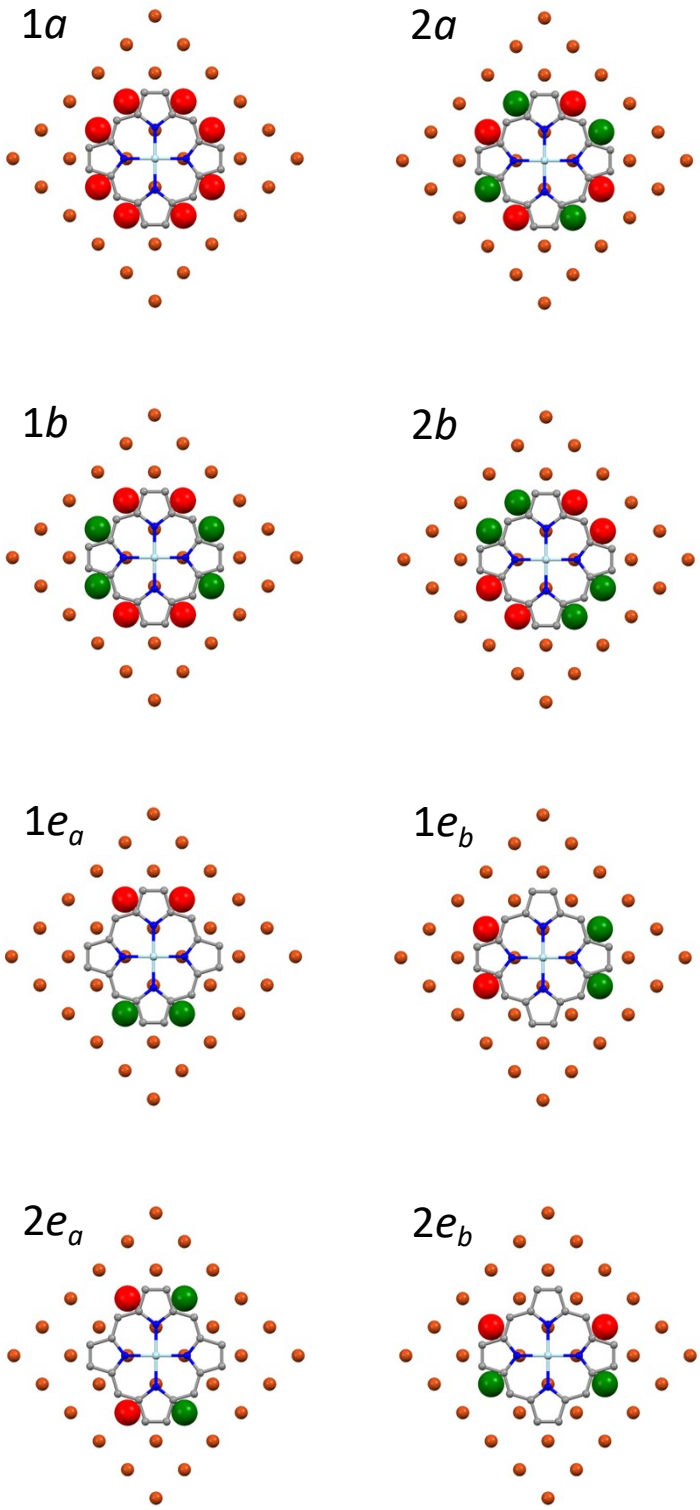

Figure S3. Schematic representation of the ${}^{nnn}Cu_{ffh}^{S}$ 4s AOs SALC of symmetry *a*, *b* and *e*. Large red and green spheres represent Cu^{S} 4s AOs and corresponding different phases. The ^{pmc}NiP planar core of the optimized D_{4h} NiTPP with the Ni–N bonds aligned with the <001> directions and the Ni species at 1.93 Å from the substrate and positioned at the *ffh* site has been superimposed to the substrate in each panel of the figure.