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Supplementary information

A Comparative XPS, UV PES, NEXAFS and DFT study of the electronic structure of the Salen ligand in the H_2(Salen) molecule and the [Ni(Salen)] complex

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As can be seen from Figure S1, all presented survey spectra of the metal-free H_2(Salen) molecule and the [Ni(Salen)] complex do not show any peaks from substrate elements or contaminant inclusions. Therefore, it can be stated that the sample layers prepared by evaporation and deposition on the Pt foil are of high purity.

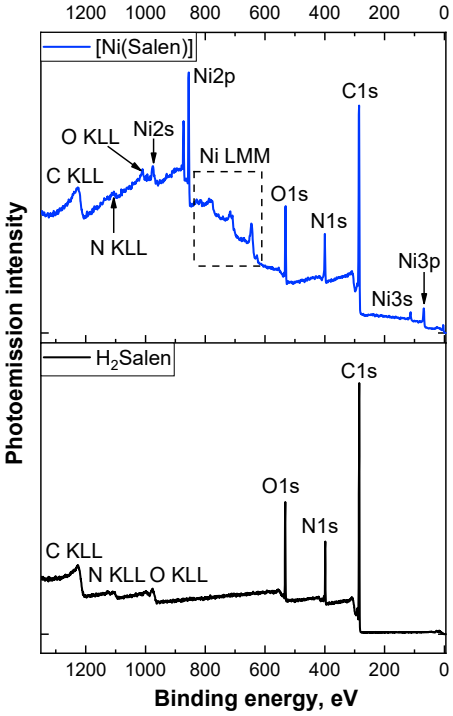

Figure S1. Overview PE spectra from the metal-free H_2Salen and [Ni(Salen)] complex deposited onto Pt foil were measured using ESCALAB 250 Xi electron spectrometer with Al Kα radiation ($h\nu$ = 1486.6 eV).

Table S1. Fitting parameters for C 1s PE spectra of H_2(Salen) and [Ni(Salen)].

Experiment					
Substance	**PE band**	**E_{bind}, eV**	**FWHM, eV**	**Relative peak intensity**	**Relative total intensity**
H_2(Salen)	Cα	284.78	1.09	1.0	1.0
	Cβ	286.16	1.25	0.47	0.52
[Ni(Salen)]	Cα	285.77	0.97	1.0	1.0
	Cβ	287.24	0.97	0.63	0.63
Calculation					
Substance	**PE band**	**E_{bind}, eV**	**FWHM, eV**	**Relative peak intensity**	**Relative total intensity**
H_2(Salen)	Cα	284.81	1.10	1.0	1.0
	Cβ1	285.59	1.0	0.165	0.165
	Cβ2	286.53	1.0	0.165	0.165
[Ni(Salen)]	Cα	285.78	0.97	1.0	1.0
	Cβ	287.49	0.97	0.60	0.60

Table S2. Calculated C 1s binding energies E_{bind} (in eV)* for different carbon atoms in the H_2(Salen) molecule and the [Ni(Salen)] complex.

Atom / **Substance**		**C1 (8)**	**C2 (2) –N**	**C3 (2) –N**	**C4 (2)**	**C5 (2) –O**
H_2(Salen)	E_{bind}	284.53—284.87	284.92	285.50	284.86	286.54
[Ni(Salen)]	E_{bind}	285.38—286.03	287.33	287.71	285.84	287.44

* The calculated C1s binding energies E_{bind} are indicated taking into account the energy shifts of 5.64 eV and 6.86 eV for H_2(Salen) and [Ni(Salen)], respectively, to ensure the energy matching of the Cα bands in the calculated and experimental C1s PE spectra.

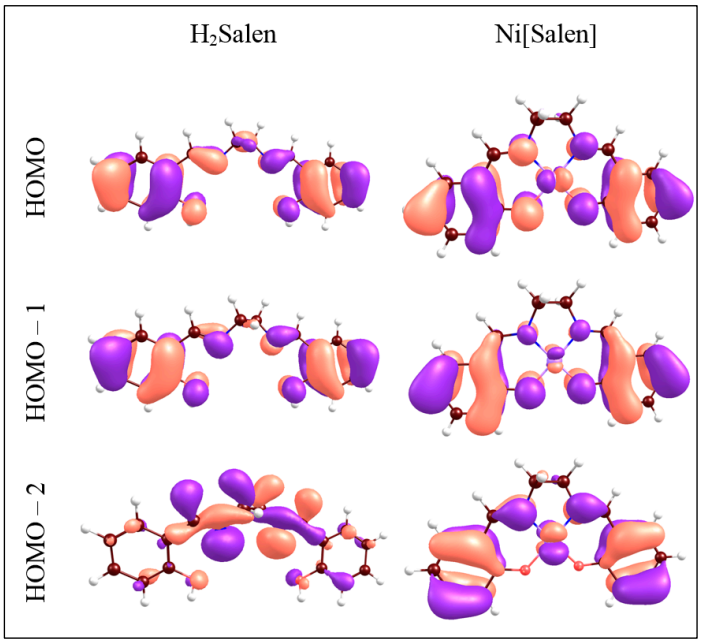

Figure S2. Higher occupied molecular orbitals of H_2(Salen) and [Ni(Salen)].

Table S3. Optimized Cartesian atomic coordinates (angstroms) of free Salen and [Ni(Salen)] complex.

H_2(Salen)				[Ni(Salen)]			
Atom	**x**	**y**	**z**	**Atom**	**x**	**y**	**z**
C	4.65588	−0.21927	−0.16965	Ni	1.1774	−2.03015	6.3E−4
C	−2.31653	−3.80039	0.1927	C	4.08562	−0.50511	0.15779
C	5.25018	−1.48792	0.01994	C	−1.75584	−3.50347	−0.15746
C	−1.64312	−5.02413	−0.02461	C	4.03458	−1.93944	0.13494
C	3.21225	0.03233	−0.30943	C	−0.56075	−4.29825	−0.13577
C	−1.66716	−2.49761	0.41145	C	2.89726	0.2611	0.01317
C	0.9276	−0.36181	−0.45957	C	−1.68541	−2.09141	−0.01001
C	−0.0025	−0.89483	0.64679	C	0.55957	0.67078	−0.33441
C	−3.72084	−3.82299	0.20277	C	−0.65548	0.04681	0.33857
C	5.50673	0.89671	−0.22374	C	−3.02257	−4.12641	−0.29615
C	−2.37846	−6.19789	−0.22188	C	5.33055	0.16107	0.29233
C	6.63941	−1.5937	0.14713	C	−0.71909	−5.71026	−0.25246
C	6.88671	0.79244	−0.09946	C	5.27472	−2.6337	0.24684
C	−4.45194	−4.98807	0.00642	C	6.50754	−0.54013	0.40646
C	7.45313	−0.46715	0.08824	C	−3.13836	−5.49113	−0.4158
C	−3.76921	−6.1841	−0.20778	C	6.46341	−1.95302	0.38039
N	−0.41952	−2.26329	0.40866	C	−1.96471	−6.27896	−0.39057
N	2.28946	−0.83916	−0.31404	N	−0.59333	−1.39548	0.07978
O	4.45636	−2.58622	0.0781	N	1.69521	−0.22074	−0.07603
O	−0.28658	−5.039	−0.03542	O	2.94679	−2.62321	0.01242
H	2.97234	1.10552	−0.41779	O	0.6289	−3.81314	−0.01065
H	−2.39115	−1.68166	0.58861	H	3.01213	1.34695	−0.03731
H	0.54388	−0.70901	−1.42554	H	−2.63464	−1.5521	0.04151
H	−0.86654	−0.2126	0.73439	H	0.39424	0.72249	−1.41685
H	0.87752	0.74128	−0.45501	H	−1.59006	0.48082	−0.03166
H	0.54429	−0.86414	1.59588	H	0.75182	1.68345	0.0351
H	−4.24284	−2.88612	0.37037	H	−0.60054	0.21281	1.42087
H	5.05555	1.87338	−0.36853	H	−3.91002	−3.49993	−0.30656
H	−1.84644	−7.13103	−0.38729	H	5.33842	1.24732	0.30308
H	7.08134	−2.57573	0.29379	H	0.18056	−6.31343	−0.23207
H	7.51026	1.67701	−0.14744	H	5.24024	−3.71628	0.22589
H	−5.53493	−4.96513	0.02035	H	7.45346	−0.0231	0.51094
H	8.52708	−0.57738	0.18943	H	−4.10964	−5.95798	−0.52396
H	−4.31445	−7.10836	−0.36332	H	7.38816	−2.51477	0.46697
H	0.01839	−5.93813	−0.20292	H	−2.04674	−7.35751	−0.48126
H	5.00499	−3.36619	0.22037				