Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for "ELECTRONIC STRUCTURE OF P-TYPE PERYLENE MONOIMIDE-BASED DONOR–ACCEPTOR DYES ON THE NICKEL OXIDE (100) SURFACE: A DFT APPROACH"

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1. SUPPLEMENTARY INFORMATIONS RELATIVE TO THE ISOLATED DYE MOLECULES

Isolated dye molecules were calculated with Gaussian09 using the B3LYP hybrid functional and the 6-31(d) basis set. We provide the optimized geometries and the minimum energies for all dye molecules in the APPENDIX 1 (Tables S2 - S9).

We also performed a scan calculation for the molecule **2** to study conformation changes due to thermal vibrations. The results presented in Fig. S1 demonstrate that the dye molecule is able to rotate ~20 degrees, because the energy required for rotation is small. However, this does not affect the energy levels, which means that the small rotation will not have an effect on the results. The B3LYP TD-DFT results are depicted in Figures S2 - S5.

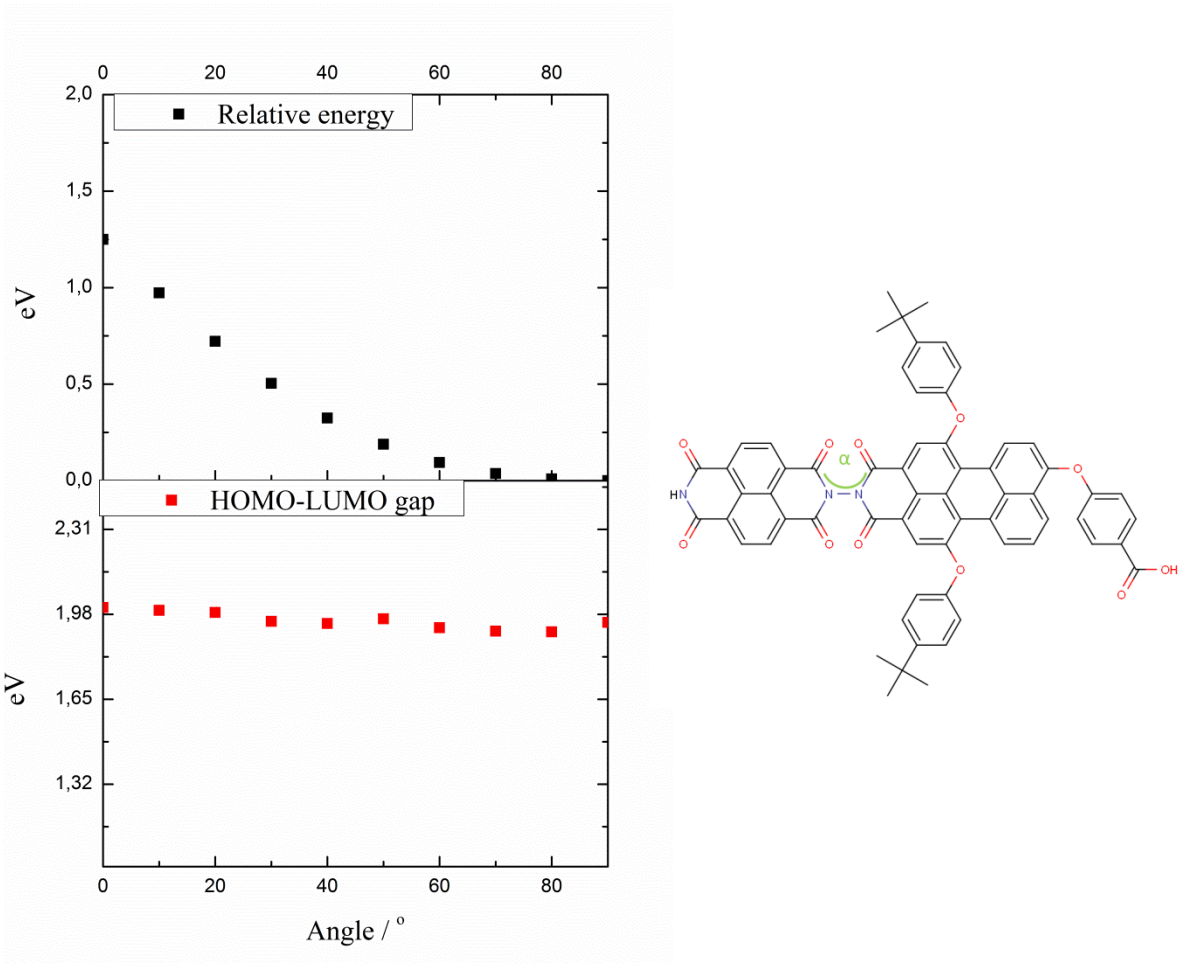

Fig S1. Potential energy scan of angle (α) in model **2** and its effect on the HOMO-LUMO gap.

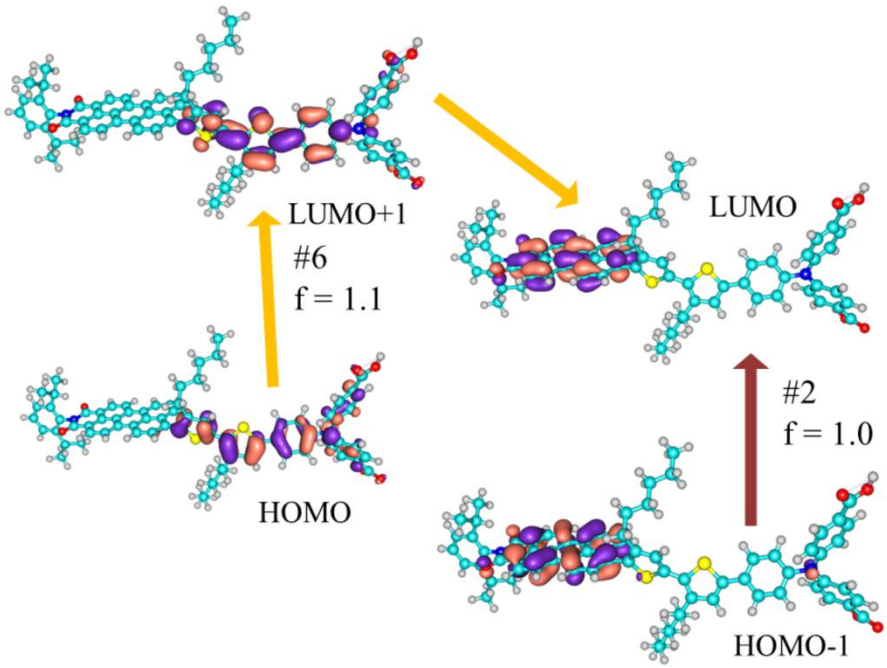

Fig. S2. Orbitals corresponding to the transitions presented in Table 1 for dye **1**. Yellow arrows demonstrate the desired transitions and the red arrow the possible but non-desired transition. Value *f* is the oscillator strength.

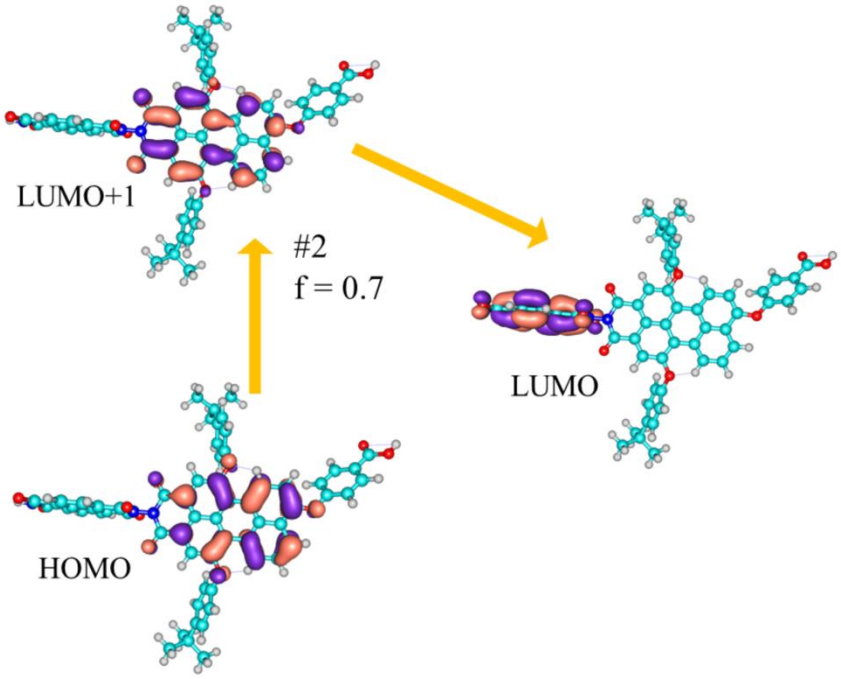

Fig. S3. Orbitals corresponding to the transitions presented in Table 1 for dye **2**. Yellow arrows demonstrate the desired transitions. Value *f* is the oscillator strength.

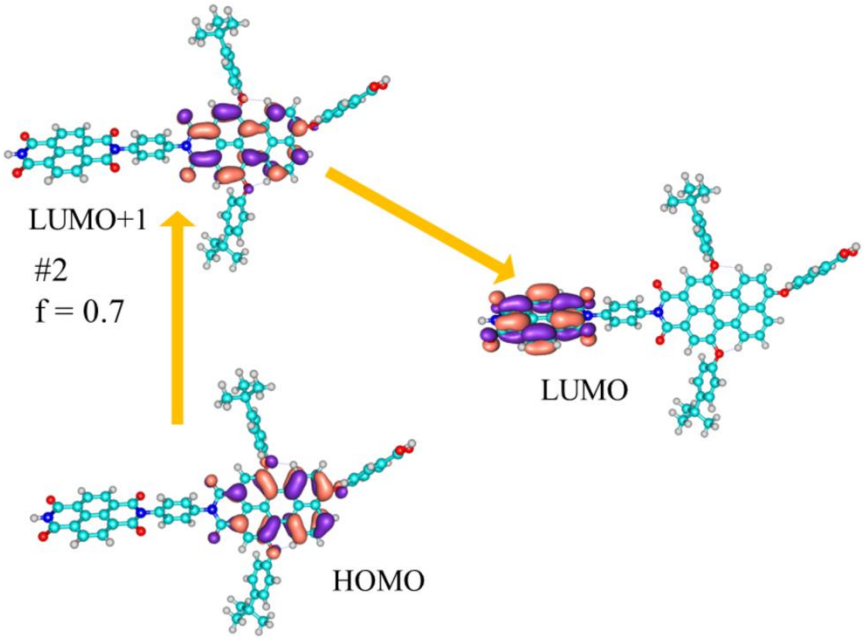

Fig. S4. Orbitals corresponding to the transitions presented in Table 1 for dye **3**. Yellow arrows demonstrate the desired transitions. Value *f* is the oscillator strength.

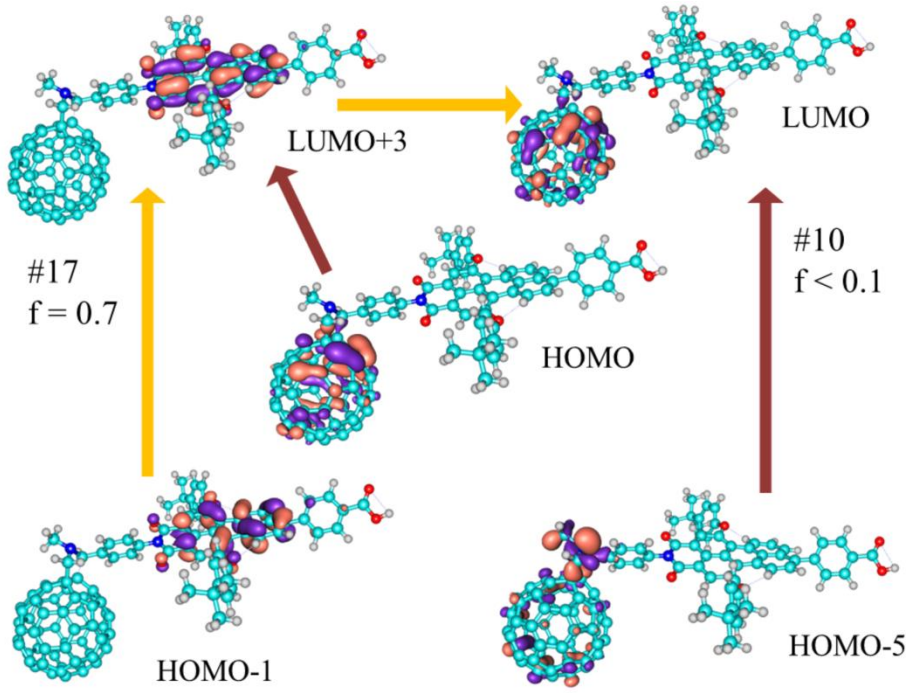

Fig. S5. Orbitals corresponding to the transitions presented in Table 1 for dye **4**. Yellow arrows demonstrate the desired transitions and the red arrows the possible but non-desired transitions. Value *f* is the oscillator strength.

We performed TDDFT calculations with CAM-B3LYP to confirm the B3LYP results. The CAM-B3LYP results are similar to the B3LYP results. The strongest excitations are from HOMO to LUMO+1 as to be expected (inside the donor). The oscillator strength (*f*) is stronger and wavelength is 20 - 50 nm shorter, but it is expected/normal according to the previous similar studies [1,2].

2. SUPPLEMENTARY INFORMATION RELATIVE TO THE SEMICONDUCTOR: THE NiO BULK AND THE NiO(100) SURFACE

NiO crystal structure and surfaces have been studied in the past both experimentally and theoretically (see Table S1) so we compare our results to the previous data. We used CRYSTAL09 program for our calculations. The B3LYP density functional was used with 86411/6411/41 and 8411/411 basis sets for Ni and O, respectively. The NiO bulk model was optimized using 65 unique k-points and the surface model contained 34 unique k-points.

Table S1. Calculated and experimental band gaps of the NiO(100) surface reported in literature in comparison with our own value.

Computation/ Experiment/	**Software / Method**	**E_g / eV**	**Slab thickness in layers**	**Reference**
Computation	MOLCAS3/ CASSCF/CASPT2	4.04/3.88		3
	Own code/(SIC)-LSD[i]	2.72		4
	CRYSTAL95/UHF	~4	1	5
	CRYSTAL98/B3LYP	3.9		6
	CRYSTAL09/B3LYP -the present work	4.0	4 (4 × 4)	this work
	VASP/HSE03	4.1		7
	VASP/PBE+U	3.02		8
Experiment	Optical abs. threshold Inversed photoemission	3.8 3.5 4.3		9 10,11 12

i. SIC-LSD: self-interaction-corrected local spin density

Following tools (keywords) were used to describe the system: EIGSHIFT, LEVSHIFT, ATOMSPIN, SPINLOCK, FMIXING, BROYDEN, and SMEAR. EIGSHIFT was used to lower the preferred Ni α or β d-orbitals to make the antiferromagnetic AF2 initial guess occupation for the first SCF cycle. LEVSHIFT increases the band gap to prevent the occupied states from mixing with the unoccupied states. Next two keywords are spin related. ATOMSPIN was used to determine the AF2 spin state. SPINLOCK was used to keep the total spin density unchanged from initial guess until 20 SCF cycles had passed. FMIXING and BROYDEN describe how much the SCF guess is allowed to change for the next cycle. The difference is that the initial FMIXING value can be changed with BROYDEN after certain amount of SCF cycles (e.g. 20–50 depending of the system) has passed. We used first higher mixing rate (90 to 80) for 20–30 cycles, after which BROYDEN changes the FMIXING value to 55. Last keyword, SMEAR, affects the occupation of the orbitals in Fermi level by adjusting the finite temperature.

The DOS and band structures of the NiO bulk and the NiO(100) surface are presented in Figures S6 - S10. Figures S6 and S7 show results for NiO bulk and Figures S8 - S10 for the NiO(100) surface. In Figure S10 the partial DOS (PDOS) of the 3d orbitals of the NiO surface demonstrates that the Ni atomic orbitals which have the e_g and t_{2g} symmetry are split so that the t_{2g} orbitals are occupied and the e_g orbitals lie on the conduction band. We do not go into deep details of the DOS and band structures of the NiO bulk and the NiO(100) surface as they and their properties have already been calculated in the previous studies (see the references in Table S1). We only note that our results are in agreement with the previously calculated and experimental results.

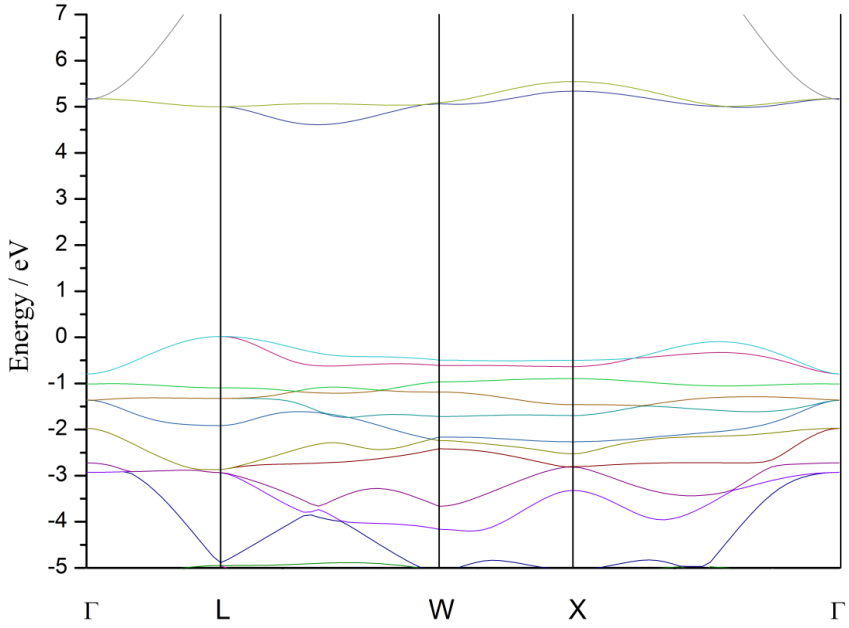

Fig. S6. The band structure of the NiO bulk.

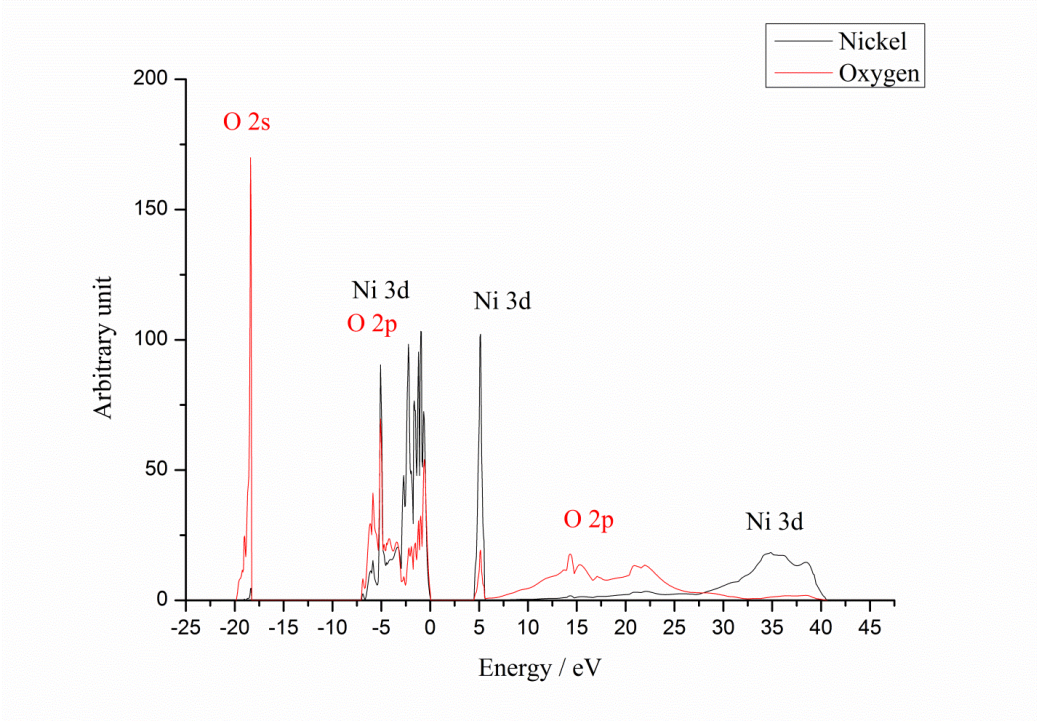

Fig S7. DOS of the bulk.

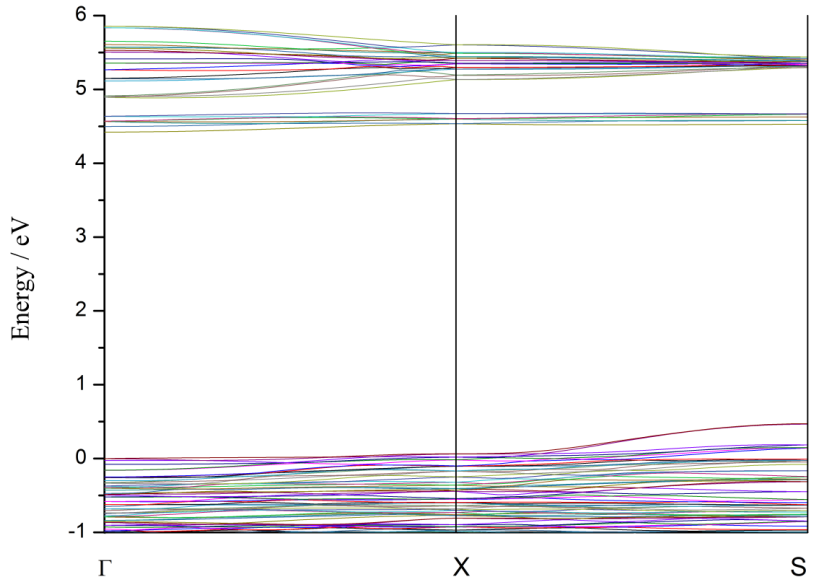

Fig S8. The band structure of the NiO(100) surface.

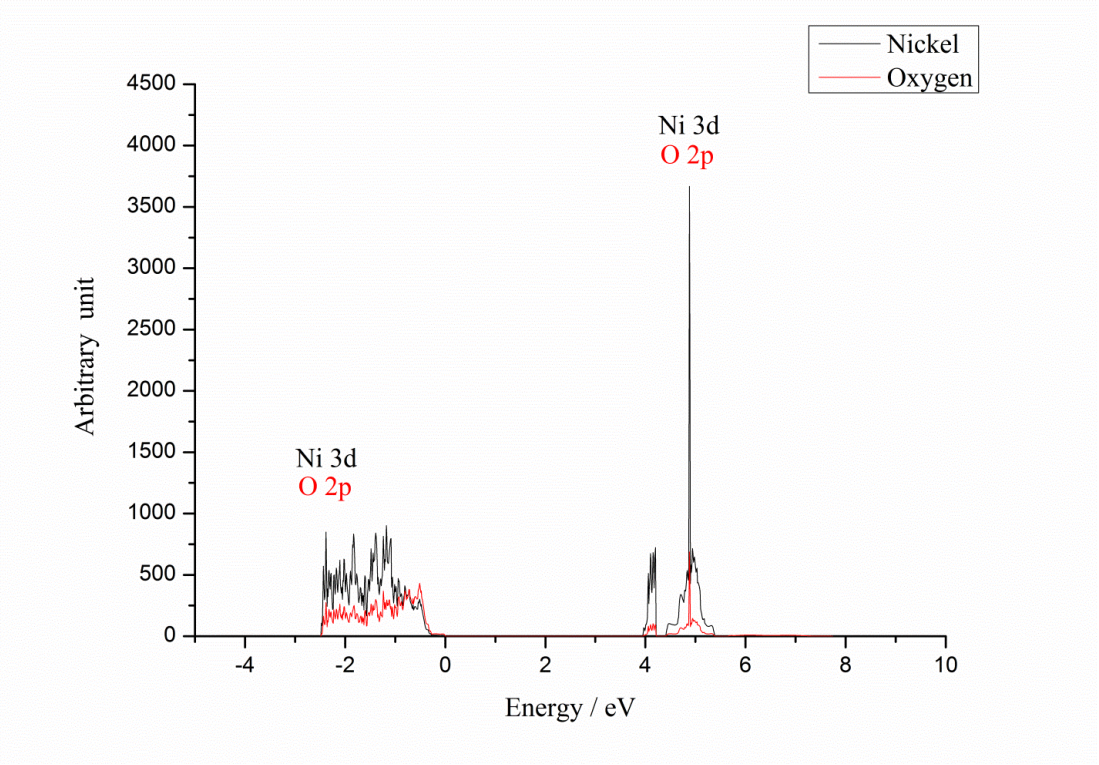

Fig S9. DOS of the NiO(100) surface.

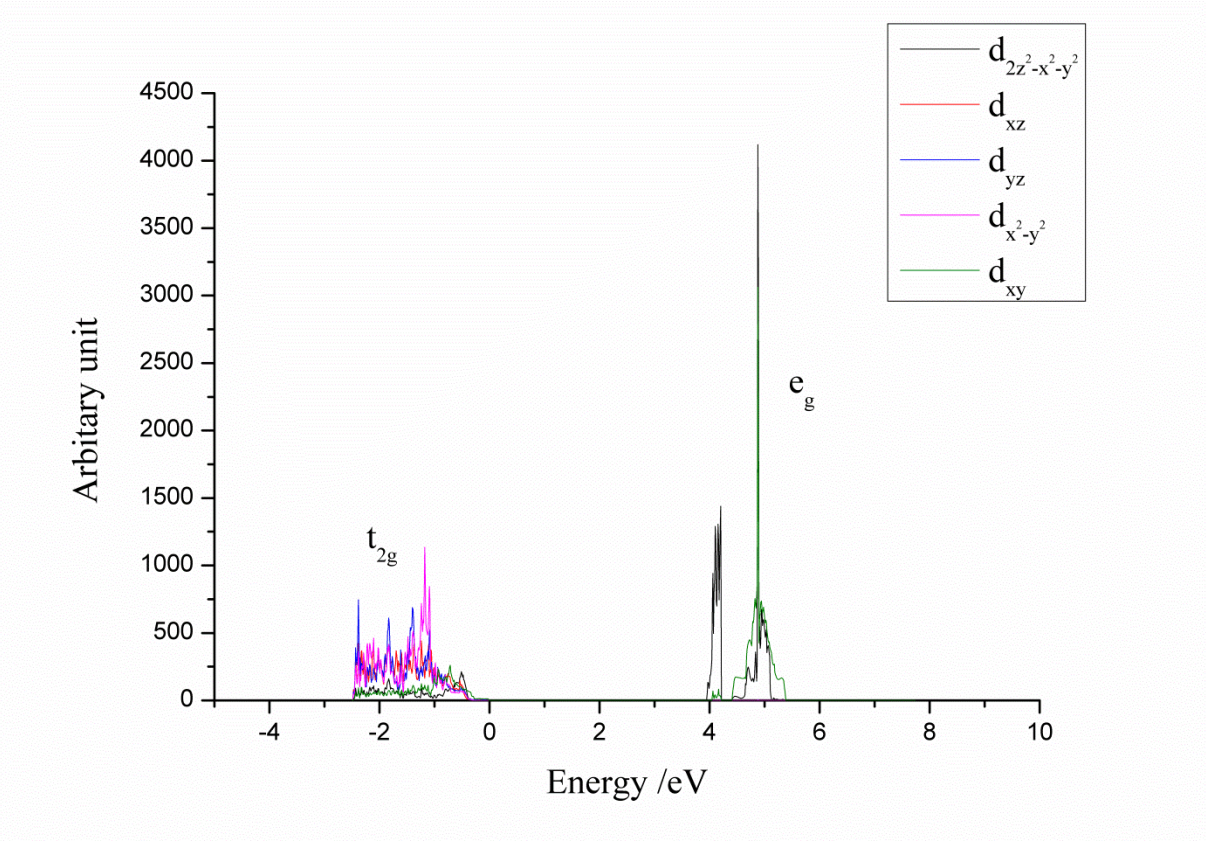

Fig S10. PDOS of the NiO(100) surface. The image shows only d-orbitals of the nickel. They are splitted as shown in Figure.

Effective Hole Mass

From our calculated band energies, we can evaluate the effective masses of charge carriers with the equation 1 of the main article. To find the second derivative we first discretize the first derivatives as

$$\frac{dE}{dk} = \frac{\Delta E}{\Delta k} = \frac{E_2 - E_1}{k_2 - k_1} = E_1'$$

and

$$\frac{dE}{dk} = \frac{\Delta E}{\Delta k} = \frac{E_3 - E_2}{k_3 - k_2} = E_3'$$

Now, the second derivative can be written as

$$\frac{d^2E}{dk^2} = \frac{E_3' - E_1'}{\Delta k} = \frac{E_3 - 2E_2 + E_1}{\Delta k^2}$$

which is the three-point equation we use here. Substitution of energies around the valence maximum yields,

$$\frac{d^2E}{dk^2} = \frac{-0.73940 - 2 * (-0.73928) + (-0.73946)}{(0.34176 - 0.32277)^2} = -0.80975$$

which finally gives the effective mass of an electron

$$m^* = \frac{1}{-0.80975} \approx -1.2$$

Now, the effective mass of the hole is of opposite sign, +1.2. All the values are from our calculations and given in atomic units.

3. SUPPLEMENTARY INFORMATION RELATIVE TO THE COMBINED SYSTEMS

All calculations were performed using CRYSTAL09. We utilized B3LYP hybrid functional with the TZVP (dye molecule **1**), 6-31G(d,p) (dye molecules **2-4**), 86411/6411/41 (surface Ni), and 8411/411 (surface O) basis sets. We provide the optimized geometry and the minimum energy of **1a**, **1b** and **2**. The combined system was calculated using only one (1) k-point.

Single point calculations with PBE0 functional were performed to study the band structures of the combined systems (Figures S11–S12). This was done to assess that the results are qualitatively the same despite the chosen functional.

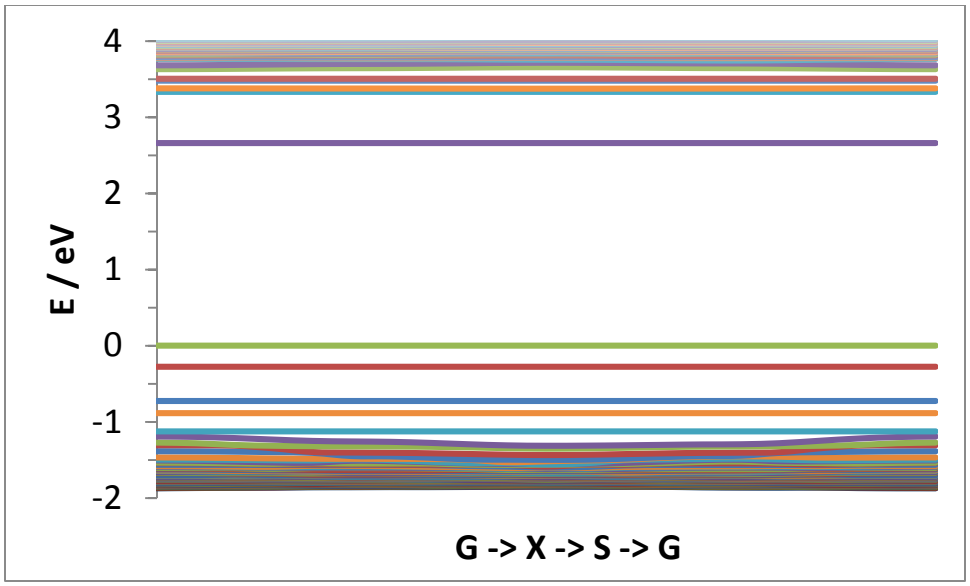

Fig. S11. Band structure of combined system **1b** with PBE0 functional.

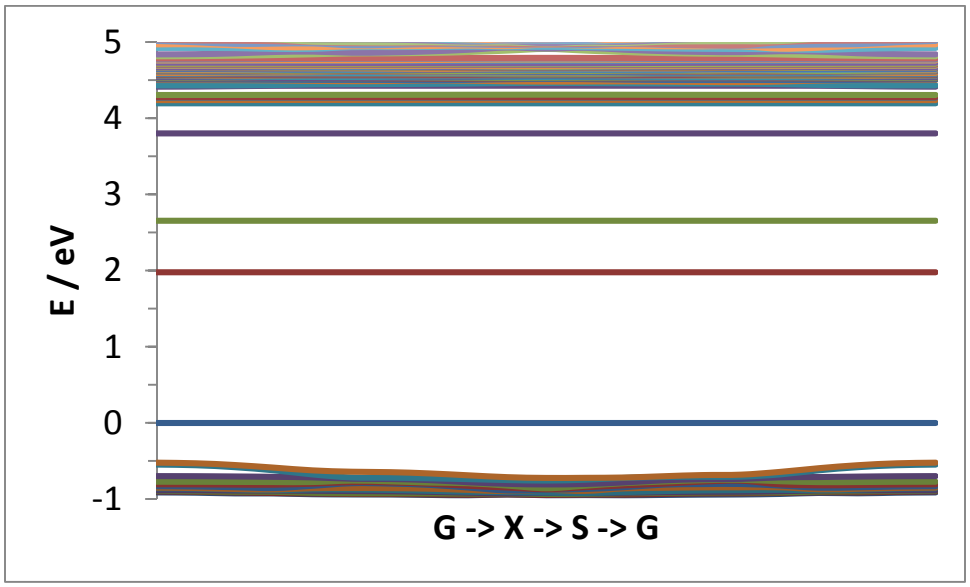

Fig. S12. Band structure of combined system **2** with PBE0 functional.

SUPPLEMENTARY INFORMATION REFERENCES

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APPENDIX 1: Coordinates of models

Table S2. The coordinates of the NiO bulk.

Energy / au	-3167.025747		
Coordinates / Å	x	y	z
Ni	0.00000	0.00000	0.00000
Ni	4.21271	4.21271	4.21271
O	2.10635	2.10635	2.10635
O	-2.10635	-2.10635	-2.10635

Table S3. Oligothiophene-trisarylamine perylene monoimide, **1**.

Energy / au	-4217.371561		
Coordinates / Å	x	y	z
C	-8.62160	0.27036	-2.16908
C	-7.22842	0.15643	-2.28000
C	-9.23506	0.12400	-0.94884
C	-8.45870	-0.15877	0.19865
C	-7.05088	-0.29210	0.09241
C	-6.42957	-0.11373	-1.18192
H	-9.23539	0.47894	-3.04048
H	-6.78799	0.28558	-3.26239
C	-9.09647	-0.31832	1.45043
C	-8.34750	-0.60528	2.56555
C	-6.95568	-0.74488	2.46798
C	-6.29087	-0.60463	1.26172
H	-8.85364	-0.72208	3.51929
H	-6.40710	-0.96605	3.37673
C	-4.95716	-0.22053	-1.28398
C	-4.19134	-0.54991	-0.12056
C	-4.82451	-0.76926	1.14455
C	-4.29481	-0.01571	-2.47567
C	-2.89608	-0.12062	-2.57294
C	-2.13121	-0.44207	-1.47897
C	-2.77714	-0.67222	-0.22237
H	-4.84347	0.24194	-3.37527
H	-2.41083	0.06125	-3.52844

C	-2.02746	-1.04498	0.92395
C	-2.65376	-1.27820	2.11789
C	-4.04876	-1.13392	2.22596
H	-4.50594	-1.32411	3.19104
H	-0.95008	-1.15152	0.83638
H	-2.07742	-1.57207	2.99095
C	-10.71056	0.25450	-0.85830
N	-11.27025	0.18673	0.42280
C	-10.56725	-0.17860	1.58026
O	-11.40987	0.42737	-1.83883
O	-11.14832	-0.35642	2.63328
C	-12.70460	0.33175	0.53964
C	-13.26109	1.59930	0.76386
C	-14.65074	1.67562	0.87713
C	-15.45352	0.54822	0.77395
C	-14.87378	-0.69175	0.55414
C	-13.49063	-0.82246	0.43333
H	-16.53261	0.63833	0.87028
H	-15.50335	-1.57556	0.47725
H	-15.10873	2.64733	1.05115
C	-12.49024	2.91549	0.84207
C	-12.22465	3.48274	-0.55968
H	-11.57885	2.82228	-1.14640
H	-11.74076	4.46405	-0.48591
H	-13.16049	3.60207	-1.11592
C	-11.21409	2.91866	1.69342
H	-13.18130	3.61144	1.33589
H	-11.34814	2.36202	2.62636
H	-10.95303	3.95251	1.94636
H	-10.35722	2.49588	1.15859
C	-12.89012	-2.19869	0.19506
C	-13.16244	-3.12870	1.38248
H	-12.77291	-2.69266	2.30835
H	-12.68271	-4.10185	1.22558
H	-14.23708	-3.30323	1.51312
C	-13.38654	-2.79375	-1.12724
H	-11.80356	-2.09327	0.11008
H	-14.47048	-2.95786	-1.10992
H	-12.90629	-3.76096	-1.31584
H	-13.15730	-2.12271	-1.96179
C	-0.65688	-0.54622	-1.61635
S	0.35670	0.77181	-1.13047
C	1.79344	-0.06018	-1.62585

C	1.47662	-1.29436	-2.12273
C	0.07668	-1.58482	-2.12617
H	2.22612	-1.98627	-2.49752
C	3.13130	0.50818	-1.44969
S	4.41820	-0.55599	-0.97358
C	5.58156	0.72413	-1.00091
C	4.98312	1.89997	-1.35351
C	3.58285	1.79417	-1.61859
H	5.52059	2.84260	-1.41440
C	-0.50032	-2.89291	-2.61355
C	-1.09524	-3.76111	-1.49515
H	0.29039	-3.45267	-3.12915
H	-1.27919	-2.69585	-3.36059
C	-0.10204	-4.13229	-0.39550
H	-1.50330	-4.67732	-1.94280
H	-1.94787	-3.23486	-1.04636
C	-0.76290	-4.88159	0.76002
H	0.37497	-3.22094	-0.00654
H	0.70898	-4.74293	-0.81976
C	0.21162	-5.26720	1.87135
H	-1.25547	-5.78775	0.37735
H	-1.56298	-4.25318	1.18035
C	-0.47081	-5.99185	3.02891
H	0.70965	-4.36171	2.24537
H	1.00554	-5.90214	1.45463
H	-1.24645	-5.36317	3.48248
H	0.24418	-6.26077	3.81362
H	-0.95328	-6.91436	2.68505
C	2.75065	2.98539	-2.01319
C	2.32144	3.83729	-0.81163
H	1.86180	2.65937	-2.56609
H	3.33396	3.61004	-2.70291
C	1.47547	5.04247	-1.21594
H	3.21578	4.17618	-0.26967
H	1.75653	3.21230	-0.10587
C	1.05274	5.90223	-0.02639
H	0.57976	4.69268	-1.75006
H	2.03797	5.66045	-1.93152
C	0.20992	7.11301	-0.42435
H	1.94864	6.24528	0.51200
H	0.48661	5.28419	0.68578
C	-0.20651	7.96190	0.77416
H	-0.68452	6.76985	-0.96220

H	0.77685	7.73028	-1.13491
H	-0.80047	7.37404	1.48390
H	-0.80885	8.82350	0.46719
H	0.67110	8.34118	1.31099
C	6.99882	0.48971	-0.67836
C	7.99153	1.30507	-1.23455
C	9.33069	1.10927	-0.93226
C	9.71418	0.08955	-0.05829
C	7.39510	-0.53463	0.18842
C	8.73305	-0.73163	0.49979
H	6.64398	-1.17132	0.65066
H	7.71237	2.08411	-1.93919
H	10.09128	1.74327	-1.38013
H	9.02433	-1.52305	1.18516
N	11.08773	-0.10963	0.25604
C	11.87474	0.99943	0.63664
C	13.21230	1.10330	0.23057
C	13.96967	2.20057	0.60539
C	13.40973	3.22033	1.37627
C	12.07530	3.12400	1.77400
C	11.31541	2.02213	1.41373
H	13.65004	0.32200	-0.38372
H	15.00584	2.29283	0.29291
H	11.63625	3.91075	2.37959
H	10.28078	1.94402	1.73441
C	11.63771	-1.40703	0.17347
C	11.19437	-2.29807	-0.81331
C	12.61784	-1.82815	1.08240
C	13.15009	-3.10507	0.99615
C	12.70389	-3.99138	0.01426
C	11.72066	-3.57702	-0.88476
H	12.95713	-1.14900	1.85890
H	11.38624	-4.27293	-1.64868
H	10.43885	-1.97814	-1.52458
H	13.90686	-3.42489	1.70571
C	13.23649	-5.36943	-0.11540
C	14.26700	4.37466	1.74038
O	13.61992	5.30644	2.47221
H	14.27495	6.00102	2.64827
O	15.43013	4.49908	1.42874
O	14.18830	-5.65829	0.79727
H	14.45578	-6.57360	0.61534
O	12.87610	-6.17628	-0.94286

Table S4. Perylene monoimide naphthalene diimide, **2**.

Energy / au	-3418.489257		
Coordinates / Å	x	y	z
C	0.37500	-1.92380	-0.67092
C	1.71972	-1.54068	-0.75141
C	-0.62219	-0.97360	-0.62990
C	-0.28831	0.40303	-0.62301
C	1.08348	0.80826	-0.66384
C	2.11325	-0.18795	-0.80918
H	0.10706	-2.97393	-0.66043
C	-1.31297	1.37855	-0.58371
C	-0.99025	2.71850	-0.58422
C	0.34887	3.12625	-0.55084
C	1.41583	2.20379	-0.54105
H	-1.78628	3.45351	-0.59741
C	3.50205	0.25079	-0.99861
C	3.83920	1.61383	-0.70990
C	2.83237	2.58970	-0.40839
C	4.51872	-0.59660	-1.44684
C	5.85569	-0.18249	-1.53468
C	6.20532	1.08756	-1.13590
C	5.21569	2.02021	-0.71739
H	4.28380	-1.60483	-1.74643
H	6.60985	-0.87064	-1.90139
C	5.57740	3.32725	-0.31426
C	4.60089	4.21544	0.07213
C	3.24490	3.85896	0.00631
H	2.51032	4.59881	0.27875
H	6.62473	3.60546	-0.31269
H	4.86893	5.21321	0.40753
C	-2.02552	-1.42908	-0.58862
N	-2.98492	-0.39095	-0.56689
C	-2.74031	1.00069	-0.56720
O	-2.37637	-2.59480	-0.57176
O	-3.66591	1.79146	-0.55062
O	7.49972	1.56393	-1.20698
C	8.57761	0.77635	-0.87441
C	8.54451	-0.17475	0.15308
C	9.70201	-0.87691	0.46559
C	10.90416	-0.63022	-0.21359

C	10.91616	0.32521	-1.24076
C	9.76106	1.02480	-1.57481
H	7.62404	-0.35879	0.69593
H	9.69726	-1.62574	1.25064
H	11.81521	0.50511	-1.82607
H	9.75485	1.75655	-2.37582
C	12.10299	-1.43498	0.17921
O	12.03345	-2.48388	0.77557
O	13.32162	-0.93332	-0.16751
H	13.23010	-0.01888	-0.47978
O	2.67406	-2.53081	-0.85053
C	2.56583	-3.68318	-0.08002
C	2.26257	-3.64623	1.27863
C	2.24854	-4.83607	2.00966
C	2.54260	-6.07295	1.41908
C	2.85188	-6.06809	0.04761
C	2.86232	-4.89508	-0.70167
H	3.08613	-7.00104	-0.45684
H	3.09840	-4.90598	-1.76129
H	2.00711	-4.77871	3.06492
H	2.04308	-2.70055	1.76408
C	2.53543	-7.39876	2.20173
C	2.19307	-7.19694	3.68994
H	2.20697	-8.16408	4.20469
H	1.19470	-6.76575	3.82553
H	2.91922	-6.54672	4.19118
C	3.93271	-8.05740	2.11457
H	4.22136	-8.26801	1.07944
H	3.94038	-9.00799	2.66162
H	4.70086	-7.40840	2.55020
C	1.48103	-8.35093	1.58855
H	1.69394	-8.57251	0.53736
H	0.47841	-7.91175	1.64089
H	1.46470	-9.30305	2.13287
O	0.62999	4.47178	-0.61979
C	-0.19026	5.40594	0.00240
C	-0.50176	6.55932	-0.71582
C	-1.24714	7.56427	-0.10542
C	-1.70395	7.45317	1.21954
C	-1.36954	6.28079	1.91130
C	-0.61628	5.26383	1.32096
H	-0.15733	6.65573	-1.74070
H	-0.36788	4.36861	1.88284

H	-1.69012	6.14194	2.93744
H	-1.48101	8.45241	-0.68533
C	-2.53500	8.58740	1.84629
C	-2.92377	8.28836	3.30671
H	-3.53744	7.38417	3.39005
H	-3.50958	9.12187	3.70996
H	-2.04267	8.16512	3.94699
C	-3.83543	8.78152	1.03037
H	-4.44047	7.86788	1.03297
H	-3.62684	9.04057	-0.01307
H	-4.43829	9.59057	1.46052
C	-1.71624	9.90007	1.82524
H	-0.79072	9.79441	2.40269
H	-2.29868	10.71958	2.26337
H	-1.44267	10.19512	0.80674
N	-4.31052	-0.78067	-0.52224
C	-4.87230	-0.92853	0.76464
C	-6.29880	-1.34199	0.78618
C	-6.99921	-1.56490	-0.42707
C	-6.36987	-1.39951	-1.68755
C	-4.94666	-0.98058	-1.76751
O	-4.21179	-0.72430	1.76343
O	-4.34742	-0.81452	-2.81043
C	-6.93619	-1.50857	2.00456
C	-8.28642	-1.90049	2.05375
C	-8.99355	-2.12568	0.88477
C	-8.36462	-1.96301	-0.37820
H	-6.37292	-1.33064	2.91431
H	-8.79476	-2.03291	3.00303
C	-9.06395	-2.18763	-1.59385
C	-8.42476	-2.02042	-2.81068
C	-7.07532	-1.62509	-2.85803
H	-8.98569	-2.19972	-3.72189
H	-6.56601	-1.49029	-3.80622
C	-10.42055	-2.53960	0.95294
N	-11.03695	-2.74014	-0.28280
C	-10.49142	-2.60408	-1.56013
O	-11.03558	-2.70050	1.99358
O	-11.16374	-2.81828	-2.55464
H	-12.01139	-3.02387	-0.24818

Table S5. Perylene monoimide phenyl naphthalene diimide, **3**.

Energy / au	-3649.56525		
Coordinates / Å	x	y	z
C	-1.51081	-1.78270	-0.91716
C	-0.70073	-0.71362	-0.60017
C	-1.27623	0.55178	-0.34921
C	-2.69464	0.73059	-0.41742
C	-3.54075	-0.41244	-0.64397
C	-2.90387	-1.63990	-0.92749
H	-1.05518	-2.73860	-1.14616
C	-0.43244	1.63838	-0.02796
C	-0.97894	2.87615	0.23170
C	-2.35962	3.08170	0.11316
C	-3.24857	2.04940	-0.25413
H	-0.32574	3.69135	0.51898
C	-5.00068	-0.23946	-0.57156
C	-5.53909	1.09058	-0.55411
C	-4.69338	2.24696	-0.46999
C	-5.89980	-1.30813	-0.52031
C	-7.28954	-1.12698	-0.51519
C	-7.81312	0.14337	-0.59051
C	-6.96071	1.28157	-0.62192
H	-5.53037	-2.31964	-0.50102
H	-7.94531	-1.99057	-0.48639
C	-7.50610	2.58386	-0.71876
C	-6.66759	3.67284	-0.74387
C	-5.28085	3.50797	-0.60393
H	-8.58175	2.69861	-0.78172
H	-7.07307	4.67558	-0.84433
H	-4.66351	4.39062	-0.59009
O	-9.16564	0.38728	-0.71954
C	-10.10041	-0.31855	0.00354
C	-11.34525	-0.49803	-0.60954
C	-12.36372	-1.13671	0.08484
C	-12.15179	-1.60323	1.39046
C	-10.90071	-1.41179	1.99426
C	-9.87418	-0.76941	1.30913
H	-11.49066	-0.13214	-1.62067
H	-13.33617	-1.28919	-0.37135
H	-10.73517	-1.76061	3.00750

H	-8.91025	-0.61272	1.78038
C	-13.27407	-2.28137	2.08156
O	-12.95527	-2.69411	3.33742
H	-13.76188	-3.11695	3.68530
O	-14.37741	-2.46653	1.60603
C	0.76301	-0.92813	-0.54672
N	1.55296	0.19431	-0.20711
C	1.03746	1.48214	0.06430
O	1.27850	-2.01172	-0.77425
O	1.78005	2.40723	0.35461
C	2.98240	0.01135	-0.12430
C	3.51623	-0.85876	0.82638
C	4.89407	-1.03925	0.90524
C	5.73424	-0.33487	0.04451
C	5.20367	0.54054	-0.90146
C	3.82453	0.70700	-0.99171
H	2.85586	-1.40050	1.49394
H	5.31543	-1.71630	1.64045
N	7.16828	-0.51290	0.13589
H	5.86437	1.08201	-1.56985
H	3.40365	1.38523	-1.72522
C	7.81002	-0.03598	1.30103
C	9.28440	-0.22879	1.37647
C	9.97868	-0.86538	0.31920
C	9.29033	-1.32780	-0.82873
C	7.81659	-1.15023	-0.94577
O	7.18067	0.50241	2.19433
O	7.19363	-1.53078	-1.92098
C	9.97259	0.21965	2.49242
C	11.36604	0.04630	2.58680
C	12.06725	-0.57486	1.56662
C	11.38705	-1.04312	0.41171
H	9.41493	0.70401	3.28672
H	11.91320	0.39411	3.45680
C	9.98403	-1.95043	-1.85396
C	11.37730	-2.12852	-1.76538
C	12.07308	-1.68382	-0.65339
H	11.92876	-2.61487	-2.56326
H	9.43101	-2.29519	-2.72103
C	13.53914	-0.75367	1.67927
N	14.14084	-1.39143	0.59295
C	13.54519	-1.87736	-0.57239
H	15.14615	-1.51864	0.65916

O	14.20146	-0.38344	2.63395
O	14.21242	-2.41567	-1.43967
O	-3.67481	-2.71554	-1.30944
O	-2.87243	4.31293	0.45532
C	-3.28275	-4.01776	-1.02304
C	-3.38208	-4.95568	-2.04442
C	-2.89797	-4.41321	0.25999
C	-2.60136	-5.75213	0.49794
C	-2.68819	-6.72844	-0.51066
C	-3.08923	-6.29593	-1.78178
H	-3.68882	-4.63216	-3.03415
H	-2.82857	-3.68127	1.05889
H	-2.29961	-6.03796	1.50149
C	-2.34860	-8.19558	-0.19160
H	-3.17483	-7.00376	-2.59830
C	-3.29939	-8.71640	0.91267
H	-3.21011	-8.13485	1.83627
H	-3.06742	-9.76092	1.15381
H	-4.34436	-8.66696	0.58587
C	-2.49711	-9.11017	-1.42228
H	-3.52371	-9.11501	-1.80615
H	-2.24288	-10.14016	-1.14836
H	-1.82740	-8.81098	-2.23658
C	-0.88624	-8.28936	0.30537
H	-0.72279	-7.69121	1.20803
H	-0.18763	-7.93433	-0.46059
H	-0.63118	-9.32904	0.54405
C	-2.16135	5.48105	0.21008
C	-1.58016	5.75668	-1.02561
C	-2.12981	6.43245	1.22849
C	-1.50686	7.65647	1.00196
C	-0.95270	6.98772	-1.22885
C	-0.89928	7.96690	-0.22726
H	-1.61246	5.01869	-1.82132
H	-2.59306	6.20309	2.18300
H	-1.49162	8.38164	1.81050
H	-0.50513	7.17419	-2.19843
C	-0.21182	9.33040	-0.42251
C	0.94513	9.47099	0.59568
H	0.58871	9.40576	1.62915
H	1.44340	10.44076	0.47557
H	1.69344	8.68364	0.45069
C	0.37258	9.49357	-1.83846

H	1.13528	8.73715	-2.05549
H	0.84923	10.47599	-1.92904
H	-0.40303	9.43128	-2.61053
C	-1.23824	10.46498	-0.19229
H	-1.66215	10.43477	0.81697
H	-2.06735	10.39404	-0.90552
H	-0.75996	11.44329	-0.32253

Table S6. Perylene monoimide phenyl fullerene, **4**.

Energy / au	-5086.177853		

Coordinates / Å	x	y	z
C	9.31636	0.97752	-1.86942
C	10.14918	1.18021	-0.76713
C	10.70347	0.06881	-0.09155
C	10.73491	0.04647	1.30622
C	10.21406	1.13960	2.04263
C	9.66965	2.23815	1.37012
C	9.63677	2.25530	-0.04249
C	8.49226	2.70620	-0.70413
C	8.29270	1.90683	-1.81382
C	9.03295	-0.31528	-2.32111
C	9.58072	-1.41408	-1.66594
C	10.42172	-1.22422	-0.53944
C	10.28542	-2.04866	0.57913
C	10.47627	-1.26308	1.72143
C	9.69560	-1.49674	2.87951
C	9.18151	-0.41737	3.60637
C	9.44157	0.90890	3.18438
C	8.42073	1.86571	3.21585
C	8.56000	2.68281	2.09301
C	7.40778	3.14594	1.40683
C	7.37961	3.15293	0.01658
C	6.08753	2.82563	-0.41556
C	5.85356	2.10395	-1.62575
C	6.98232	1.57939	-2.25101
C	6.69700	0.34083	-2.81020
C	7.73856	-0.63667	-2.74723
C	7.48330	-1.94218	-2.33847
C	8.62433	-2.42251	-1.66880
C	8.49182	-3.26119	-0.53775
C	9.31458	-3.07644	0.58021
C	8.54697	-3.30980	1.72470
C	8.73778	-2.51476	2.88210
C	7.63207	-2.06512	3.61136
C	7.90621	-0.76845	4.05790
C	6.87449	0.20262	4.08980
C	7.13008	1.51042	3.66953
C	5.99747	1.97626	2.99009

C	6.13655	2.79951	1.84913
C	5.31714	2.60208	0.72125
C	4.35195	1.57761	0.72685
C	4.05554	0.83491	-0.43060
C	4.61428	1.20640	-1.82310
C	5.21762	-0.02718	-2.62929
C	5.12630	-1.39239	-1.92319
C	6.20138	-2.29726	-1.88068
C	6.08256	-3.10876	-0.75448
C	7.22401	-3.60361	-0.08364
C	7.25468	-3.64032	1.31240
C	6.13861	-3.18587	2.04930
C	6.32373	-2.40522	3.19209
C	5.31006	-1.44472	3.22137
C	5.58628	-0.13569	3.67215
C	5.05128	0.95958	2.98942
C	4.24003	0.75850	1.84958
C	3.97442	-0.52024	1.40707
C	4.50757	-1.63174	2.09495
C	5.01615	-2.70093	1.37537
C	4.99447	-2.66132	-0.03388
C	4.44421	-1.57253	-0.71879
C	3.92481	-0.48784	0.00984
H	-5.06733	-5.20687	1.85643
H	-2.20938	-8.56183	0.33275
H	-3.98325	-7.26394	1.14490
C	-4.87851	-5.37066	0.80226
C	-4.25558	-6.54761	0.38529
H	5.77935	2.34543	-4.44700
H	-3.83105	-9.36226	0.22111
C	-2.93800	-9.04079	-0.35719
O	-5.84338	-3.26559	0.29841
H	4.98746	1.72257	-5.94159
C	4.80725	2.17880	-4.94473
C	-5.24126	-4.39848	-0.12812
N	3.90500	1.32105	-4.16046
C	-4.00307	-6.78151	-0.98865
H	-2.45969	-9.95624	-0.76734
H	-3.51955	-2.52724	-0.49106
H	-6.09562	8.97952	2.67716
O	-1.70346	-1.13698	-1.22621
C	4.44104	-0.03110	-3.94127
C	-4.24455	-1.72352	-0.47686

C	-5.56283	-2.00607	-0.11455
C	-3.33357	-8.07237	-1.49715
H	-0.21338	2.66934	-0.16073
C	-10.62400	1.95442	1.06615
H	-7.62356	9.52790	1.90536
H	-1.33331	-7.17629	-1.61536
C	-2.48542	-0.20078	-1.15180
C	-9.33218	2.23216	0.61017
H	-11.24267	2.79603	1.34595
C	-3.82985	-0.43798	-0.77650
H	2.16012	2.95030	-0.74947
C	0.18391	2.14677	-1.02098
H	-9.09463	3.27128	0.58220
C	-6.51731	9.64153	1.89227
C	1.54147	2.29754	-1.35284
C	-6.55166	-0.96512	-0.06887
C	-11.10812	0.64547	1.19426
C	-4.99716	-4.61069	-1.48885
C	-4.39172	-5.78914	-1.91632
C	-8.39747	1.20818	0.28761
C	-2.04826	-7.71414	-2.27493
C	-8.84455	-0.13556	0.43722
C	-6.11946	0.37657	-0.30174
C	-10.21768	-0.41339	0.81646
C	-7.94493	-1.22056	0.20154
C	-4.74619	0.62076	-0.67114
H	-1.55167	-8.63162	-2.65739
H	4.32553	3.16442	-5.11968
H	-6.26983	10.68821	2.16987
N	-2.04132	1.08374	-1.39950
C	-0.64369	1.29358	-1.77041
C	-7.03683	1.47227	-0.17359
C	-10.66927	-1.74304	0.75760
C	2.09990	1.62764	-2.46265
C	-8.48609	-2.53579	0.20917
C	-4.28780	1.91989	-0.93457
C	3.58764	1.85913	-2.81579
C	-9.81919	-2.77201	0.44989
C	-2.92355	2.14471	-1.28705
C	-6.54140	2.78307	-0.50833
C	-0.09200	0.62108	-2.87551
C	1.25110	0.80406	-3.23438
H	-5.24351	-9.07971	-1.87533

C	-6.18254	5.46994	0.73285
C	-5.19154	2.97312	-0.86923
H	-5.80662	4.69257	1.38569
C	-4.31552	-8.81503	-2.42793
H	-7.93974	-3.41372	-0.03803
H	-5.28955	-3.86446	-2.21717
C	-5.84974	6.79711	0.98658
H	-10.20354	-3.78310	0.39488
H	-5.21726	7.01061	1.83623
O	-2.53663	3.28058	-1.52100
C	-7.01470	5.14293	-0.34333
H	-4.22712	-5.92370	-2.97588
C	-6.33286	7.83668	0.16204
O	-7.36819	3.85553	-0.57727
H	-0.71354	-0.03008	-3.47701
C	-7.50369	6.15516	-1.17139
C	-5.96251	9.29587	0.49324
C	-7.16166	7.48967	-0.93328
H	-3.93852	8.79887	1.23378
H	-3.86019	-9.75144	-2.81537
H	1.61451	0.28964	-4.11024
H	-2.26285	-7.06752	-3.15094
H	-4.85055	3.96747	-1.13028
H	-8.14487	5.90729	-2.00880
H	-7.55991	8.23656	-1.60337
C	-4.42679	9.45982	0.48803
H	-4.60103	-8.19473	-3.30298
H	-7.65848	10.26969	-0.52578
H	-4.14304	10.50444	0.74028
C	-6.54819	10.31654	-0.51102
H	-6.26341	11.35312	-0.22771
H	-4.01346	9.21600	-0.51429
H	-6.16095	10.12986	-1.53615
H	5.00441	-0.45530	-4.80238
H	3.56223	-0.69334	-3.80099
H	3.68632	2.96986	-2.80833
H	-11.69544	-2.01553	0.89425
C	-12.52748	0.43631	1.76415
C	-13.53665	1.41190	1.57079
C	-12.88060	-0.70106	2.54331
C	-14.83505	1.23051	2.07538
C	-15.17714	0.07086	2.78338
C	-14.18572	-0.88964	3.01916

H	-13.34002	2.31262	1.01108
H	-15.58222	1.99303	1.89548
H	-12.15421	-1.45117	2.81331
H	-14.41570	-1.78425	3.58840
C	-16.56601	-0.12388	3.28737
O	-17.46574	0.88222	3.20505
O	-16.90046	-1.19171	3.78188
H	-18.36333	0.78611	3.55631

Table S7. Oligothiophene-trisarylamine perylene monoimide, **1** (two binding points) with NiO (100) surface.

Energy / au	-206904.407890		
Coordinates / Å	x	y	z
Ni	-0.05007	-4.83708	3.30022
Ni	-5.94565	1.15564	3.12673
Ni	6.02758	1.13139	3.18381
Ni	0.01583	7.12630	3.12951
Ni	-0.01405	-1.83118	3.12484
Ni	-5.94129	4.11551	3.12794
Ni	6.01438	4.20903	3.17138
Ni	0.02393	10.10271	3.12865
Ni	-0.02197	1.17245	3.12324
Ni	6.02560	-4.87014	3.13825
Ni	-5.92818	-4.76906	3.15288
Ni	0.02444	-10.75024	3.13103
Ni	0.02450	4.17375	3.29496
Ni	6.03407	-1.77321	3.15370
Ni	-5.94382	-1.81093	3.13463
Ni	0.00526	-7.77570	3.13151
Ni	-2.97785	1.15677	3.12586
Ni	2.89952	-4.87459	3.14496
Ni	2.99577	7.14636	3.12997
Ni	8.97831	1.17307	3.13729
Ni	2.92528	-1.77078	3.14368
Ni	-2.95018	4.13495	3.13036
Ni	-2.95522	-7.76132	3.13810
Ni	-8.91948	-1.80948	3.12907
Ni	2.92494	1.12553	3.14313
Ni	-2.94595	7.11712	3.13006
Ni	-2.91792	-4.78070	3.42384
Ni	-8.91991	1.15740	3.12823
Ni	-2.97503	-1.82794	3.13362
Ni	2.98778	-7.80450	3.12569
Ni	2.86770	4.22944	3.35096
Ni	8.97843	-1.81822	3.13206
O	-4.46303	-0.31840	3.14947
O	1.51983	-6.33579	3.11444
O	1.50250	5.71368	3.07148
O	7.47295	-0.33170	3.16268

O	1.55786	-3.28794	3.14805
O	-4.46188	2.65522	3.14751
O	7.45330	2.64139	3.18341
O	1.49987	8.63063	3.14519
O	1.48940	-0.33295	3.14349
O	-4.45433	5.62220	3.14363
O	-4.45899	-6.28894	3.16929
O	-10.41540	-0.32603	3.14525
O	1.50216	2.58576	3.09339
O	7.43750	-3.30998	3.17318
O	-4.47511	-3.28281	3.14764
O	1.50488	-9.27730	3.14688
O	-1.48176	-0.32220	3.14778
O	4.48143	-6.27260	3.16882
O	4.49297	5.63682	3.17489
O	10.43792	-0.33042	3.15238
O	-1.50664	2.63907	3.12979
O	4.49860	-3.30877	3.60699
O	-7.43672	-3.29364	3.15336
O	-1.47412	-9.28074	3.14963
O	4.48612	-0.34599	3.20067
O	-1.50211	5.65766	3.12449
O	-1.49148	-6.34955	3.08342
O	-7.43927	-0.32116	3.14806
O	-1.47331	-3.25366	3.08596
O	-7.43196	2.65105	3.14997
O	4.52720	2.59608	3.56971
O	-1.48250	8.61851	3.15048
Ni	-4.45722	-0.33841	1.04892
Ni	1.48011	-6.29682	1.05105
Ni	1.50084	5.62341	1.05403
Ni	7.46430	-0.32750	1.05404
Ni	1.48267	-3.32626	1.07071
Ni	-4.45306	2.64169	1.04683
Ni	7.45522	2.65259	1.07460
Ni	1.50408	8.60444	1.04907
Ni	1.48831	-0.32891	1.04332
Ni	-4.44468	5.61885	1.04527
Ni	-4.43693	-6.26559	1.08656
Ni	-10.41205	-0.33362	1.04631
Ni	1.49148	2.66902	1.07143
Ni	7.45964	-3.31596	1.05600
Ni	-4.43906	-3.32582	1.07535

Ni	1.49984	-9.27281	1.04639
Ni	-1.48496	-0.33980	1.04982
Ni	4.47624	-6.29736	1.05639
Ni	4.47112	5.62595	1.09032
Ni	10.44171	-0.33123	1.05047
Ni	-1.47034	2.65492	1.05855
Ni	4.47629	-3.30841	0.96770
Ni	-7.42708	-3.30897	1.05438
Ni	-1.47826	-9.26407	1.05219
Ni	4.48114	-0.32685	1.07386
Ni	-1.46608	5.61822	1.05603
Ni	-1.48965	-6.27081	1.06615
Ni	-7.43320	-0.33521	1.04685
Ni	-1.48696	-3.33611	1.06477
Ni	-7.43414	2.64004	1.04379
Ni	4.46066	2.66950	1.00301
Ni	-1.47453	8.60338	1.04728
O	0.02744	-4.80548	1.05807
O	-5.94713	1.15915	1.04438
O	5.93886	1.17271	1.11286
O	0.00342	7.12958	1.03745
O	0.02929	-1.81460	1.04290
O	-5.94783	4.14144	1.04848
O	5.94057	4.10140	1.10668
O	0.00583	10.09582	1.04576
O	0.01161	1.14597	1.04068
O	5.92879	-4.78108	1.06956
O	-5.94791	-4.80873	1.06525
O	0.00863	-10.76268	1.04769
O	0.00486	4.14122	1.05639
O	5.94061	-1.84948	1.10020
O	-5.94765	-1.81991	1.04739
O	0.01352	-7.79572	1.03997
O	-2.96953	1.15712	1.04184
O	3.02593	-4.77448	1.08582
O	2.99889	7.12502	1.04375
O	8.93648	1.14886	1.05989
O	3.03038	-1.84318	1.08826
O	-2.97493	4.13895	1.04348
O	-2.98460	-7.79681	1.05327
O	-8.92525	-1.81926	1.04490
O	3.02632	1.16427	1.08658
O	-2.98184	7.12289	1.05039

O	-2.97412	-4.80290	1.03739
O	-8.92383	1.15640	1.04509
O	-2.97113	-1.81368	1.04127
O	2.99660	-7.78092	1.04480
O	3.01690	4.11756	1.10286
O	8.93260	-1.82133	1.05733
Ni	0.00627	-4.80642	-1.05330
Ni	-5.94474	1.14959	-1.06917
Ni	5.96756	1.15662	-1.05293
Ni	0.01283	7.11057	-1.06429
Ni	0.00578	-1.83130	-1.05871
Ni	-5.94676	4.12881	-1.06672
Ni	5.97299	4.14337	-1.04518
Ni	0.01290	10.08957	-1.06646
Ni	0.00776	1.15573	-1.06039
Ni	5.97176	-4.81210	-1.07389
Ni	-5.94530	-4.80437	-1.04632
Ni	0.01111	-10.76218	-1.06573
Ni	0.00994	4.13278	-1.05546
Ni	5.97085	-1.82104	-1.06668
Ni	-5.94214	-1.82932	-1.06142
Ni	0.00674	-7.78317	-1.06249
Ni	-2.96627	1.15125	-1.06456
Ni	2.98257	-4.81144	-1.06734
Ni	2.99380	7.11261	-1.05699
Ni	8.94716	1.15748	-1.05648
Ni	2.98221	-1.82240	-1.06397
Ni	-2.96463	4.13029	-1.06561
Ni	-2.96952	-7.77947	-1.05043
Ni	-8.92256	-1.82671	-1.06640
Ni	2.98465	1.15509	-1.05751
Ni	-2.96471	7.10940	-1.06474
Ni	-2.96989	-4.80508	-1.05334
Ni	-8.92422	1.15087	-1.06925
Ni	-2.96877	-1.83124	-1.05976
Ni	2.98807	-7.78699	-1.06648
Ni	2.98557	4.14164	-1.05021
Ni	8.94854	-1.82611	-1.06170
O	-4.45677	-0.33343	-1.07252
O	1.50644	-6.29009	-1.06344
O	1.50403	5.61961	-1.06231
O	7.44448	-0.33620	-1.04230
O	1.51319	-3.31323	-1.05702

O	-4.45759	2.64704	-1.07081
O	7.44551	2.63751	-1.04528
O	1.49933	8.60284	-1.07029
O	1.51340	-0.33533	-1.05349
O	-4.46369	5.62697	-1.06512
O	-4.46494	-6.30153	-1.04909
O	-10.41624	-0.33497	-1.07051
O	1.50975	2.64380	-1.05519
O	7.44686	-3.31022	-1.05534
O	-4.45979	-3.31547	-1.06562
O	1.50039	-9.27265	-1.07045
O	-1.47449	-0.33580	-1.06999
O	4.47727	-6.28690	-1.06551
O	4.48004	5.61393	-1.04777
O	10.42985	-0.33546	-1.06309
O	-1.47726	2.64526	-1.06861
O	4.48079	-3.31206	-1.06677
O	-7.43453	-3.31443	-1.06645
O	-1.48386	-9.27554	-1.06305
O	4.48244	-0.33751	-1.04276
O	-1.48133	5.62578	-1.06883
O	-1.47804	-6.29671	-1.06722
O	-7.43567	-0.33488	-1.07186
O	-1.47404	-3.31491	-1.06882
O	-7.43473	2.64537	-1.07116
O	4.48080	2.63877	-1.04759
O	-1.48455	8.60539	-1.06753
Ni	-4.45589	-0.34801	-3.14600
Ni	1.49448	-6.30360	-3.14218
Ni	1.50181	5.61399	-3.13843
Ni	7.45775	-0.34016	-3.13366
Ni	1.49446	-3.32475	-3.13820
Ni	-4.45559	2.63108	-3.14656
Ni	7.45672	2.63982	-3.12825
Ni	1.50344	8.59083	-3.14433
Ni	1.49625	-0.34304	-3.13754
Ni	-4.45693	5.60824	-3.14779
Ni	-4.45766	-6.29910	-3.13026
Ni	-10.41654	-0.34721	-3.14882
Ni	1.49972	2.63826	-3.13418
Ni	7.45936	-3.32382	-3.14158
Ni	-4.45712	-3.32566	-3.13893
Ni	1.49812	-9.28209	-3.14637

Ni	-1.47974	-0.34681	-3.14228
Ni	4.47534	-6.30731	-3.14692
Ni	4.48057	5.61610	-3.12937
Ni	10.43480	-0.34393	-3.14212
Ni	-1.47687	2.63387	-3.14320
Ni	4.47599	-3.32385	-3.14768
Ni	-7.43277	-3.32481	-3.14045
Ni	-1.48163	-9.27851	-3.13921
Ni	4.47690	-0.34067	-3.13310
Ni	-1.47658	5.61141	-3.14457
Ni	-1.48212	-6.30041	-3.13829
Ni	-7.43517	-0.34832	-3.14837
Ni	-1.48153	-3.32604	-3.14007
Ni	-7.43586	2.63144	-3.14759
Ni	4.47855	2.64051	-3.13120
Ni	-1.47608	8.59206	-3.14349
O	0.01389	-4.81140	-3.16661
O	-5.94587	1.14711	-3.17572
O	5.96538	1.14521	-3.15020
O	0.01073	7.10405	-3.17029
O	0.01713	-1.83208	-3.16509
O	-5.94680	4.12960	-3.17213
O	5.96613	4.12048	-3.15026
O	0.00728	10.08455	-3.17156
O	0.01739	1.14584	-3.16451
O	5.96944	-4.80511	-3.16637
O	-5.94774	-4.81724	-3.15915
O	0.00893	-10.76713	-3.16717
O	0.01379	4.12471	-3.16704
O	5.96579	-1.82967	-3.15922
O	-5.94630	-1.83479	-3.17279
O	0.00852	-7.79074	-3.16921
O	-2.96490	1.14737	-3.17315
O	2.99322	-4.80758	-3.16578
O	2.99096	7.10051	-3.16486
O	8.94067	1.14541	-3.15682
O	2.99349	-1.83056	-3.16015
O	-2.96774	4.12864	-3.17155
O	-2.97380	-7.79407	-3.15878
O	-8.92607	-1.83314	-3.17308
O	2.99440	1.14580	-3.15452
O	-2.96928	7.10909	-3.16562
O	-2.97008	-4.81559	-3.16746

O	-8.92457	1.14805	-3.17237
O	-2.96568	-1.83452	-3.17102
O	2.98867	-7.78778	-3.17264
O	2.99381	4.12192	-3.15642
O	8.93963	-1.82927	-3.16280
C	-1.32146	-4.39752	5.84389
O	-2.51862	-4.51153	5.43566
H	-3.06175	-3.22735	7.63698
C	-2.02891	-2.95683	7.81613
C	-1.03404	-3.54875	7.04643
C	0.29375	-3.20605	7.28521
H	1.05744	-3.68888	6.69340
H	1.64171	-1.92176	8.34934
C	0.61517	-2.23406	8.20115
C	-0.38689	-1.57782	8.90256
C	-1.71080	-1.98652	8.75077
H	-2.48731	-1.48826	9.31791
N	-0.01275	-0.38350	9.60460
H	-1.27029	0.29069	7.41129
C	-0.37641	0.88108	7.56181
C	0.39153	0.66180	8.70058
C	1.55073	1.40536	8.89448
H	2.15215	1.22848	9.77775
H	-0.61215	2.02315	5.77326
C	-0.00107	1.83066	6.64600
C	1.16046	2.57716	6.82814
C	1.93637	2.35168	7.95656
C	1.45569	3.58254	5.75961
H	2.84404	2.92414	8.10634
O	2.66247	3.76480	5.36480
O	0.43442	4.14225	5.27258
C	-8.66632	0.53740	27.42543
C	-8.18285	0.65816	26.13075
C	-8.51524	-0.63832	28.12082
C	-7.83838	-1.72079	27.52524
C	-7.32776	-1.59737	26.20614
C	-7.53961	-0.38713	25.49041
H	-9.17207	1.36291	27.90847
H	-8.31456	1.60486	25.62532
C	-7.68635	-2.93296	28.22653
C	-7.03220	-3.98577	27.63311
C	-6.50462	-3.85973	26.35610
C	-6.61611	-2.68608	25.63043

H	-6.93410	-4.91131	28.18478
H	-5.99903	-4.71532	25.93056
C	-7.07821	-0.29075	24.10381
C	-6.29865	-1.34543	23.55125
C	-6.02972	-2.52932	24.29617
C	-7.38428	0.79061	23.30438
C	-6.92011	0.89242	21.99580
C	-6.12358	-0.07942	21.44468
C	-5.78937	-1.22333	22.22696
H	-8.01047	1.58659	23.68365
H	-7.18414	1.75708	21.39871
C	-4.98996	-2.25865	21.69895
C	-4.71181	-3.36849	22.44285
C	-5.23256	-3.50241	23.72954
H	-4.98770	-4.39609	24.28705
H	-4.60012	-2.14959	20.69679
H	-4.08441	-4.15328	22.03745
C	-9.03810	-0.74086	29.49246
N	-8.73448	-1.92216	30.18825
C	-8.20949	-3.08154	29.59330
O	-9.68468	0.15130	30.02489
O	3.73793	7.77533	30.20628
C	-9.08790	-1.98665	31.59764
C	-8.13004	-1.60987	32.54505
C	-8.50502	-1.68490	33.88075
C	-9.76178	-2.10976	34.25898
C	1.23301	9.44187	33.30101
C	1.54972	9.49510	31.94972
H	1.89213	9.75882	35.31021
H	0.24722	9.10934	33.60369
H	-7.78693	-1.40023	34.64197
C	-6.71213	-1.12505	32.24712
C	-6.63598	0.20575	31.49066
H	-6.86685	0.10257	30.43225
H	-5.62297	0.60862	31.55609
H	-7.31813	0.94448	31.90884
C	-5.79862	-2.17728	31.60856
H	-6.28705	-0.92672	33.23589
H	-5.88304	-3.13955	32.11137
H	-4.75830	-1.85213	31.67750
H	-6.01100	-2.33486	30.55301
C	0.50653	9.08455	30.92608
C	0.12089	7.61195	31.08973

H	0.99497	6.96668	31.01799
H	-0.58969	7.31145	30.31736
H	-0.35164	7.42700	32.05527
C	-0.71869	10.00064	30.98692
H	0.94074	9.19406	29.93159
H	-1.22874	9.92331	31.94799
H	-1.44038	9.73100	30.21347
H	-0.43784	11.04263	30.84226
C	-5.69036	0.04337	20.04279
S	-4.06057	0.60289	19.64718
C	-4.42133	0.52986	17.91237
C	-5.69551	0.08916	17.72672
C	-6.42497	-0.17793	18.91490
H	-6.12426	-0.01276	16.73810
C	-3.43883	0.83658	16.90156
S	-3.39877	-0.19654	15.45672
C	-2.10671	0.78119	14.75098
C	-1.77635	1.79184	15.59537
C	-2.51624	1.84133	16.80652
H	-0.99390	2.50296	15.36038
C	-7.84687	-0.68148	18.92372
C	-7.98735	-2.11072	19.46275
H	-8.24675	-0.62712	17.90800
H	-8.46813	-0.01776	19.53108
C	-7.18822	-3.15145	18.68594
H	-9.04651	-2.38584	19.46847
H	-7.66717	-2.11933	20.50530
C	-7.12876	-4.50171	19.39252
H	-6.17167	-2.77769	18.53140
H	-7.61459	-3.27049	17.68358
C	5.53416	6.34503	18.60317
H	3.76988	7.06381	19.60452
H	-6.64802	-4.36482	20.36700
C	5.56379	4.99270	19.29864
H	-5.35738	-5.23014	18.41688
H	5.07625	6.23689	17.61471
H	6.02526	5.06042	20.28539
H	6.12712	4.25546	18.72505
H	4.55674	4.59560	19.43807
C	-2.27278	2.89801	17.84553
C	-1.00476	2.65147	18.67162
H	-3.13349	2.96856	18.51225
H	-2.18587	3.86968	17.34789

C	-0.71119	3.77188	19.66245
H	-0.15456	2.52525	17.99388
H	-1.10122	1.70008	19.20315
C	0.57078	3.55923	20.46058
H	-1.55611	3.87926	20.35083
H	-0.64763	4.72356	19.12299
C	0.86487	4.68431	21.44702
H	1.41481	3.45229	19.77006
H	0.51080	2.60856	21.00102
C	2.15271	4.48000	22.22987
H	0.02523	4.78289	22.14215
H	0.91246	5.63513	20.90611
H	2.12860	3.55138	22.80234
H	2.32719	5.29351	22.93479
H	3.01938	4.43034	21.56827
C	-1.57348	0.47464	13.43237
C	-1.18309	1.49917	12.57063
C	-0.68150	1.23230	11.31670
C	-0.54868	-0.08364	10.87493
C	-1.43776	-0.83806	12.98041
C	-0.92975	-1.11713	11.73242
H	-1.70420	-1.65534	13.64088
H	-1.31316	2.52865	12.88363
H	-0.40868	2.04432	10.65653
H	-0.81335	-2.14324	11.40938
O	-0.28909	-4.87331	5.27329
H	4.47011	-3.32457	4.57473
H	4.29528	2.73545	4.50808

Table S8. Oligothiophene-trisarylamine perylene monoimide, **1** (one binding point) with NiO (100) surface.

Energy / au	-206104.566183		
Coordinates / Å	x	y	z
Ni	0.00452	-4.39894	3.19293
Ni	-5.90951	1.49832	3.17887
Ni	5.93225	1.48905	3.18078
Ni	-0.00441	7.41951	3.18853
Ni	0.01354	-1.43340	3.26374
Ni	-5.91049	4.45155	3.17869
Ni	5.92738	4.45563	3.18576
Ni	0.00319	10.36356	3.18307
Ni	-0.05872	1.40763	3.23968
Ni	5.90823	-4.41120	3.18081
Ni	-5.89541	-4.40146	3.18300
Ni	0.00569	-10.31069	3.18748
Ni	-0.07097	4.50370	3.19550
Ni	5.92093	-1.46511	3.17342
Ni	-5.90446	-1.45296	3.17981
Ni	0.00499	-7.35895	3.18379
Ni	-2.96538	1.49262	3.17986
Ni	2.95775	-4.41164	3.17933
Ni	2.95983	7.42110	3.18875
Ni	8.87087	1.49869	3.18179
Ni	2.96420	-1.47253	3.17166
Ni	-2.97238	4.45453	3.17984
Ni	-2.94380	-7.35895	3.18149
Ni	-8.85643	-1.45004	3.18446
Ni	3.03024	1.41519	3.18535
Ni	-2.95875	7.41165	3.18346
Ni	-2.94600	-4.40487	3.18246
Ni	-8.85736	1.50131	3.18411
Ni	-2.95229	-1.45896	3.18064
Ni	2.95540	-7.36148	3.17705
Ni	3.01204	4.50812	3.20747
Ni	8.86613	-1.45463	3.17697
O	-4.44221	0.02098	3.18166
O	1.48299	-5.89019	3.18974
O	1.47843	5.92706	3.21306
O	7.39705	0.01898	3.18536

O	1.50269	-2.95201	3.19212
O	-4.43826	2.97870	3.18750
O	7.39325	2.97354	3.19135
O	1.48004	8.88368	3.19642
O	1.54578	0.02514	3.17167
O	-4.43068	5.93228	3.18195
O	-4.42518	-5.88752	3.19097
O	-10.33432	0.02182	3.18795
O	1.50557	2.98696	3.31538
O	7.39186	-2.93236	3.18422
O	-4.43379	-2.93510	3.18696
O	1.48249	-8.83854	3.18432
O	-1.54060	0.01540	3.15468
O	4.43534	-5.88828	3.18100
O	4.44080	5.93435	3.19551
O	10.34289	0.02180	3.18422
O	-1.49586	2.99651	3.20112
O	4.44626	-2.93825	3.18267
O	-7.38151	-2.93140	3.19157
O	-1.47346	-8.83846	3.18667
O	4.46388	0.00896	3.17987
O	-1.48424	5.94101	3.18748
O	-1.47242	-5.88797	3.19238
O	-7.38473	0.02144	3.18716
O	-1.48983	-2.94268	3.19330
O	-7.38304	2.97510	3.18791
O	4.44158	2.97181	3.20001
O	-1.47261	8.88470	3.19188
Ni	-4.43136	0.01539	1.08310
Ni	1.47991	-5.88936	1.08624
Ni	1.47882	5.92930	1.09643
Ni	7.39342	0.01492	1.08100
Ni	1.48010	-2.93924	1.09299
Ni	-4.43339	2.96994	1.08303
Ni	7.39326	2.97025	1.08563
Ni	1.48004	8.88039	1.08877
Ni	1.48252	0.00536	1.09379
Ni	-4.43094	5.92410	1.08272
Ni	-4.42269	-5.88841	1.08665
Ni	-10.33310	0.01850	1.08571
Ni	1.47519	2.96145	1.08060
Ni	7.38863	-2.93801	1.08065
Ni	-4.42631	-2.93669	1.08523

Ni	1.48039	-8.84227	1.08383
Ni	-1.48296	0.00864	1.09092
Ni	4.43247	-5.89116	1.08178
Ni	4.43848	5.92831	1.09021
Ni	10.34332	0.01817	1.08429
Ni	-1.48500	2.96623	1.09380
Ni	4.43640	-2.94202	1.08010
Ni	-7.37970	-2.93419	1.08668
Ni	-1.47079	-8.84186	1.08479
Ni	4.44386	0.00694	1.08061
Ni	-1.48124	5.92771	1.08710
Ni	-1.47085	-5.88750	1.08851
Ni	-7.38193	0.01754	1.08394
Ni	-1.47063	-2.93457	1.09572
Ni	-7.38253	2.97037	1.08243
Ni	4.44320	2.96775	1.09169
Ni	-1.47321	8.87927	1.08494
O	0.00406	-4.41467	1.08996
O	-5.90868	1.49335	1.08215
O	5.91615	1.49154	1.08569
O	0.00363	7.39990	1.09266
O	0.00620	-1.46164	1.09536
O	-5.90607	4.44663	1.08174
O	5.91146	4.44620	1.09056
O	0.00418	10.35374	1.08627
O	0.00412	1.49461	1.09994
O	5.91264	-4.41474	1.08120
O	-5.90528	-4.41488	1.08735
O	0.00430	-10.32030	1.08554
O	0.00951	4.44348	1.10617
O	5.91711	-1.46274	1.07975
O	-5.90802	-1.46146	1.08343
O	0.00368	-7.36745	1.08597
O	-2.95975	1.49588	1.08332
O	2.95952	-4.41716	1.08241
O	2.95598	7.39932	1.09359
O	8.86674	1.49302	1.08356
O	2.96703	-1.46519	1.08264
O	-2.95372	4.44927	1.08571
O	-2.94891	-7.36733	1.08586
O	-8.85877	-1.46052	1.08666
O	2.96184	1.49590	1.09681
O	-2.94913	7.40137	1.08427

O	-2.95148	-4.41506	1.08632
O	-8.85859	1.49294	1.08408
O	-2.95844	-1.46415	1.08226
O	2.95613	-7.36823	1.08250
O	2.95192	4.44116	1.10691
O	8.86710	-1.46054	1.08264
Ni	0.00374	-4.41611	-1.03777
Ni	-5.90521	1.48908	-1.04303
Ni	5.91319	1.48876	-1.04049
Ni	0.00353	7.39583	-1.03683
Ni	0.00340	-1.46605	-1.03285
Ni	-5.90506	4.44298	-1.04437
Ni	5.91214	4.44331	-1.03741
Ni	0.00436	10.35052	-1.04152
Ni	0.00106	1.48726	-1.03145
Ni	5.91040	-4.41858	-1.04429
Ni	-5.90277	-4.41702	-1.03899
Ni	0.00441	-10.32358	-1.04228
Ni	0.00219	4.43992	-1.03296
Ni	5.91235	-1.46565	-1.04488
Ni	-5.90417	-1.46419	-1.04181
Ni	0.00385	-7.36945	-1.04114
Ni	-2.95217	1.48816	-1.03900
Ni	2.95640	-4.41808	-1.04276
Ni	2.95692	7.39629	-1.03588
Ni	8.86632	1.48998	-1.04285
Ni	2.95710	-1.46646	-1.04002
Ni	-2.95213	4.44201	-1.04037
Ni	-2.94809	-7.36945	-1.04046
Ni	-8.85716	-1.46352	-1.04101
Ni	2.95723	1.48812	-1.03544
Ni	-2.94998	7.39583	-1.04098
Ni	-2.94844	-4.41613	-1.03886
Ni	-8.85755	1.48965	-1.04291
Ni	-2.95026	-1.46521	-1.03925
Ni	2.95606	-7.37030	-1.04319
Ni	2.95695	4.44081	-1.03258
Ni	8.86573	-1.46396	-1.04376
O	-4.42942	0.01267	-1.04390
O	1.47971	-5.89380	-1.04318
O	1.48056	5.91678	-1.03087
O	7.38923	0.01303	-1.04456
O	1.48093	-2.94048	-1.04084

O	-4.42830	2.96698	-1.04380
O	7.38766	2.96699	-1.04106
O	1.48013	8.87191	-1.03859
O	1.48151	0.01415	-1.03625
O	-4.42589	5.91987	-1.04297
O	-4.42747	-5.89412	-1.04035
O	-10.33401	0.01240	-1.04211
O	1.48142	2.96593	-1.02427
O	7.38935	-2.94046	-1.04526
O	-4.42884	-2.94139	-1.04254
O	1.47954	-8.84697	-1.04342
O	-1.47391	0.01320	-1.03909
O	4.43364	-5.89421	-1.04449
O	4.43164	5.91779	-1.03460
O	10.34183	0.01293	-1.04286
O	-1.47207	2.96672	-1.03506
O	4.43564	-2.94101	-1.04569
O	-7.38194	-2.94176	-1.04038
O	-1.47282	-8.84663	-1.04291
O	4.43552	0.01379	-1.04117
O	-1.47079	5.91802	-1.03669
O	-1.47330	-5.89322	-1.04130
O	-7.38197	0.01226	-1.04350
O	-1.47350	-2.94005	-1.03993
O	-7.38146	2.96660	-1.04501
O	4.43292	2.96679	-1.03408
O	-1.47137	8.87276	-1.04103
Ni	-4.42526	0.00720	-3.13710
Ni	1.48028	-5.89757	-3.13733
Ni	1.48138	5.91296	-3.12917
Ni	7.38870	0.00829	-3.13832
Ni	1.47997	-2.94469	-3.13410
Ni	-4.42553	2.96023	-3.13634
Ni	7.38855	2.96224	-3.13466
Ni	1.48165	8.86674	-3.13275
Ni	1.47973	0.00725	-3.13094
Ni	-4.42595	5.91382	-3.14229
Ni	-4.42546	-5.89799	-3.13364
Ni	-10.33298	0.00770	-3.14239
Ni	1.48063	2.95964	-3.12834
Ni	7.38859	-2.94641	-3.13990
Ni	-4.42518	-2.94553	-3.13612
Ni	1.48061	-8.85177	-3.13920

Ni	-1.47149	0.00719	-3.13206
Ni	4.43325	-5.89879	-3.14481
Ni	4.43432	5.91400	-3.13033
Ni	10.34183	0.00812	-3.14345
Ni	-1.47205	2.95923	-3.13107
Ni	4.43358	-2.94576	-3.14011
Ni	-7.37926	-2.94663	-3.13475
Ni	-1.47193	-8.85128	-3.13854
Ni	4.43378	0.00808	-3.13556
Ni	-1.47175	5.91240	-3.13486
Ni	-1.47202	-5.89712	-3.13572
Ni	-7.37973	0.00722	-3.13996
Ni	-1.47163	-2.94452	-3.13400
Ni	-7.37955	2.96155	-3.13709
Ni	4.43456	2.96120	-3.13065
Ni	-1.47090	8.86716	-3.13396
O	0.00213	-4.42097	-3.14594
O	-5.90474	1.48430	-3.14897
O	5.90851	1.48626	-3.14474
O	0.00426	7.38837	-3.14161
O	0.00298	-1.46696	-3.14378
O	-5.90328	4.43840	-3.14828
O	5.90747	4.43771	-3.14382
O	0.00359	10.34324	-3.14642
O	0.00489	1.48742	-3.13907
O	5.91186	-4.42193	-3.14346
O	-5.90644	-4.42394	-3.14457
O	0.00331	-10.32947	-3.14242
O	0.00560	4.43618	-3.13801
O	5.90998	-1.46754	-3.15022
O	-5.90562	-1.46992	-3.14870
O	0.00177	-7.37501	-3.14906
O	-2.94946	1.48531	-3.14499
O	2.95635	-4.42103	-3.14647
O	2.95501	7.38830	-3.14065
O	8.86330	1.48535	-3.14554
O	2.95602	-1.46626	-3.14634
O	-2.94804	4.43778	-3.14425
O	-2.95190	-7.37510	-3.14794
O	-8.85840	-1.47086	-3.14632
O	2.95499	1.48779	-3.13932
O	-2.94725	7.39024	-3.13992
O	-2.95186	-4.42188	-3.14633

O	-8.85772	1.48397	-3.14230
O	-2.95098	-1.46830	-3.14648
O	2.95534	-7.37570	-3.15139
O	2.95465	4.43626	-3.13711
O	8.86429	-1.46961	-3.15059
H	0.07161	-9.95559	5.81496
H	7.87006	-1.94570	23.19986
C	-0.04665	-7.53854	14.14668
C	-0.07222	-6.28862	13.50792
C	0.49200	-7.65545	15.41313
C	1.06305	-6.51986	16.04753
C	1.09304	-5.26151	15.37498
C	0.44865	-5.12594	14.09389
H	-0.46145	-8.40800	13.66392
C	1.61243	-6.64308	17.34585
C	2.15362	-5.54253	17.97511
C	2.25063	-4.30959	17.30352
C	1.77421	-4.14951	15.98631
H	2.54462	-5.64784	18.97806
C	0.36359	-3.78712	13.49086
C	1.19928	-2.73817	14.00448
C	1.96351	-2.90781	15.20502
C	-0.48851	-3.47483	12.42859
C	-0.45558	-2.23346	11.78042
C	0.48382	-1.29584	12.13902
C	1.32134	-1.50424	13.27296
H	-1.18594	-4.21614	12.06229
H	-1.11142	-2.04397	10.93862
C	2.25731	-0.52569	13.68306
C	3.04549	-0.74596	14.79105
C	2.88465	-1.91942	15.55585
H	3.50665	-2.04968	16.42353
H	2.34252	0.38782	13.11529
H	3.76657	-0.00928	15.11838
C	0.48143	-8.99267	16.05512
N	1.05813	-9.01834	17.34915
C	1.63125	-7.93283	18.05639
O	0.03654	-10.00088	15.54299
O	2.12895	-8.11586	19.14971
O	0.61667	-0.08164	11.49402
C	0.54754	-0.04071	10.11034
C	1.01608	-1.09547	9.31811
C	0.87352	-1.02262	7.94213

C	0.34579	0.11822	7.32524
C	-0.05953	1.19029	8.12611
C	0.02060	1.11149	9.52288
H	1.45935	-1.96763	9.78699
H	1.15548	-1.86338	7.30896
H	-0.45784	2.08277	7.65417
H	-0.38712	1.88641	10.15618
C	0.18164	0.13343	5.82303
O	0.10826	-1.00649	5.29763
O	0.11962	1.28558	5.25748
O	-0.70838	-6.22359	12.27743
C	-0.37176	-7.12857	11.27650
C	0.93352	-7.58417	11.07880
C	1.20084	-8.43145	10.00070
C	0.19693	-8.87008	9.12146
C	-1.10597	-8.37875	9.35294
C	-1.39621	-7.53165	10.42419
H	-1.91593	-8.69430	8.71530
H	-2.40676	-7.18037	10.59596
H	2.22799	-8.76066	9.85809
H	1.74296	-7.21382	11.70230
C	0.45227	-9.84773	7.95997
C	-9.85906	1.65212	7.77953
H	-9.72656	1.00349	6.90314
H	-9.44958	1.13172	8.64467
H	-9.26974	2.55872	7.60874
C	-0.06631	-9.24341	6.63407
H	-1.13294	-9.00704	6.67507
H	0.46485	-8.33190	6.36791
C	-0.28831	-11.17501	8.24366
H	10.44124	0.79959	8.30179
H	0.03900	-11.59605	9.19263
H	11.71742	-0.08800	7.45107
O	2.71503	-3.21302	17.98212
C	3.75217	-3.34726	18.91165
C	3.50278	-2.82514	20.20403
C	4.51920	-2.88447	21.15692
C	5.79967	-3.45258	20.85012
C	6.00854	-3.98579	19.55047
C	4.99808	-3.93137	18.58344
H	2.54940	-2.34940	20.42401
H	5.15350	-4.37463	17.60037
H	6.94426	-4.46506	19.29248

H	4.33744	-2.43303	22.13239
C	6.90911	-3.46524	21.93030
C	-3.57866	7.71473	21.40808
H	-3.69278	6.63721	21.18295
H	-2.78264	7.78483	22.17007
H	-3.19738	8.24093	20.49594
C	6.40607	-4.29883	23.17384
H	6.21915	-5.35171	22.91800
H	5.47445	-3.87171	23.60794
H	7.18215	-4.28063	23.95455
C	7.18220	-1.98572	22.36176
H	7.61310	-1.40463	21.52752
H	6.26765	-1.47002	22.66163
N	1.14394	-10.25488	17.96656
C	-9.48996	0.82514	17.71140
C	-9.34025	-0.44528	18.48362
C	-10.36558	-0.86540	19.37301
C	-11.51339	-0.06662	19.59491
C	0.11703	-10.57630	18.87974
O	-8.64780	1.25016	16.95156
O	-0.82902	-9.84201	19.04984
C	-8.24192	-1.25457	18.25494
C	-8.08089	-2.46570	18.96401
C	2.76504	8.92422	19.86065
C	1.60156	9.71432	20.06999
H	-7.47035	-0.88119	17.59200
H	-7.21491	-3.08911	18.82181
C	0.57576	9.29292	20.95156
C	-0.53697	10.09099	21.14886
C	11.12616	-0.50272	20.46011
H	-1.30650	9.74235	21.82901
H	10.26061	0.12906	20.60834
C	2.94171	7.64470	20.58332
N	1.88772	7.29171	21.41103
C	0.74580	8.02739	21.71621
O	3.91565	6.93198	20.50247
O	-0.01847	7.63870	22.57303
H	2.07116	6.50094	22.04043
H	1.37051	2.77282	4.24352

Table S9. Perylene monoimide naphthalene diimide, **2** with NiO (100) surface.

Energy / au	-206105.208680		
Coordinates / Å	x	y	z
Ni	3.14167	-3.11801	3.15938
Ni	-5.20864	-3.13226	3.14654
Ni	3.16796	5.23843	3.14949
Ni	-5.21811	5.23550	3.15310
Ni	1.04518	-1.02617	3.37067
Ni	-7.29792	-1.04530	3.14682
Ni	1.07576	7.33072	3.15336
Ni	-7.29711	7.31932	3.14714
Ni	-1.00230	0.92332	3.31756
Ni	7.32561	1.04511	3.14739
Ni	-1.02650	-7.29441	3.15059
Ni	7.32551	-7.30011	3.14704
Ni	-3.18645	3.12761	3.17709
Ni	5.24764	3.13562	3.14369
Ni	-3.11803	-5.21501	3.14820
Ni	5.23662	-5.21080	3.14789
Ni	-3.12636	-1.05318	3.14807
Ni	5.24093	-1.04308	3.14993
Ni	-3.12829	7.32904	3.15453
Ni	5.24398	7.32080	3.14687
Ni	3.16075	1.03012	3.14439
Ni	-5.22027	1.03390	3.15122
Ni	3.15537	-7.29645	3.14943
Ni	-5.20939	-7.29924	3.14815
Ni	1.14262	3.13910	3.14904
Ni	-7.30131	3.13597	3.14672
Ni	1.06452	-5.21407	3.15436
Ni	-7.29575	-5.21508	3.14572
Ni	-1.02252	-3.13674	3.14997
Ni	7.32408	-3.12889	3.14649
Ni	-1.02627	5.29937	3.19178
Ni	7.32706	5.22861	3.14627
O	-3.12790	-3.14032	3.16389
O	5.24121	-3.13122	3.16636
O	-3.11493	5.22207	3.19682
O	5.24392	5.22983	3.16681
O	3.17648	-1.04063	3.15631

O	-5.21387	-1.04545	3.16709
O	3.15383	7.31685	3.17122
O	-5.20780	7.31501	3.17213
O	1.10030	1.10261	3.10550
O	-7.29730	1.04856	3.16674
O	1.06297	-7.30676	3.17243
O	-7.29480	-7.30529	3.16548
O	-1.03465	3.19877	3.58827
O	7.32852	3.13942	3.16554
O	-1.03186	-5.22585	3.16800
O	7.32602	-5.21779	3.16649
O	-1.06879	-1.09699	3.10131
O	7.32872	-1.04148	3.16653
O	-1.02887	7.32559	3.17711
O	7.32724	7.31579	3.16678
O	-3.14191	1.05629	3.16700
O	5.24726	1.05230	3.16469
O	-3.11997	-7.30653	3.17107
O	5.24001	-7.30446	3.16735
O	3.17254	3.14840	3.16002
O	-5.21890	3.14131	3.16918
O	3.15360	-5.21897	3.16857
O	-5.20958	-5.22061	3.16663
O	1.06233	-3.15335	3.16363
O	-7.29595	-3.13146	3.16601
O	1.06062	5.22714	3.19282
O	-7.29482	5.22750	3.16905
Ni	-3.11735	-3.13380	1.05722
Ni	5.22998	-3.13084	1.05801
Ni	-3.11868	5.21910	1.07589
Ni	5.23690	5.22129	1.05377
Ni	3.12939	-1.04609	1.07500
Ni	-5.21024	-1.04764	1.05473
Ni	3.14906	7.31284	1.05642
Ni	-5.20922	7.30977	1.05745
Ni	1.05419	1.02388	1.07383
Ni	-7.29813	1.04109	1.05436
Ni	1.05871	-7.30573	1.05877
Ni	-7.29747	-7.30881	1.05354
Ni	-1.02568	3.11457	0.98442
Ni	7.32327	3.13082	1.05221
Ni	-1.02913	-5.22123	1.05686
Ni	7.32075	-5.22025	1.05382

Ni	-1.01676	-1.04463	1.06854
Ni	7.32076	-1.04630	1.05397
Ni	-1.03020	7.31007	1.06142
Ni	7.32289	7.31043	1.05323
Ni	-3.10938	1.03429	1.08226
Ni	5.23585	1.03992	1.05363
Ni	-3.11991	-7.30866	1.05786
Ni	5.23453	-7.30663	1.05478
Ni	3.15047	3.12865	1.05003
Ni	-5.20807	3.12841	1.05631
Ni	3.14371	-5.21601	1.05976
Ni	-5.20868	-5.22152	1.05421
Ni	1.05626	-3.11600	1.08078
Ni	-7.29817	-3.13417	1.05341
Ni	1.06124	5.22602	1.06753
Ni	-7.29687	5.22039	1.05536
O	3.14813	-3.13718	1.05974
O	-5.21162	-3.13656	1.05401
O	3.14332	5.21995	1.06153
O	-5.20353	5.21628	1.06577
O	1.06023	-1.04733	1.05171
O	-7.29791	-1.04576	1.05486
O	1.05323	7.30526	1.06690
O	-7.29535	7.30677	1.05678
O	-1.03694	1.07860	1.10853
O	7.32461	1.04468	1.05438
O	-1.03244	-7.31792	1.05988
O	7.32219	-7.31159	1.05514
O	-3.08389	3.13522	1.10877
O	5.23658	3.13519	1.05188
O	-3.12253	-5.22787	1.05570
O	5.23420	-5.22357	1.05529
O	-3.12978	-1.04768	1.05176
O	5.23669	-1.04455	1.05381
O	-3.11603	7.30165	1.06810
O	5.23383	7.30818	1.05635
O	3.15703	1.05350	1.04680
O	-5.20906	1.04755	1.05960
O	3.14512	-7.31248	1.05830
O	-5.20849	-7.31439	1.05731
O	1.02445	3.14748	1.08337
O	-7.29367	3.13291	1.05647
O	1.05627	-5.22611	1.05861

O	-7.29781	-5.22408	1.05454
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O	7.32205	-3.13477	1.05416
O	-1.03123	5.18011	1.11511
O	7.32395	5.22061	1.05497
Ni	3.14141	-3.13426	-1.06322
Ni	-5.20938	-3.13711	-1.07139
Ni	3.14540	5.21923	-1.06868
Ni	-5.20853	5.21775	-1.06482
Ni	1.05758	-1.05073	-1.05909
Ni	-7.29905	-1.04914	-1.07241
Ni	1.05830	7.30796	-1.06587
Ni	-7.29796	7.30626	-1.07149
Ni	-1.03205	1.02948	-1.06224
Ni	7.32085	1.03904	-1.07280
Ni	-1.03213	-7.31288	-1.06688
Ni	7.32062	-7.31182	-1.07262
Ni	-3.12532	3.12524	-1.06660
Ni	5.23334	3.12751	-1.07307
Ni	-3.12040	-5.22437	-1.06958
Ni	5.23126	-5.22277	-1.07062
Ni	-3.12024	-1.04965	-1.06352
Ni	5.22898	-1.04856	-1.06769
Ni	-3.12190	7.30483	-1.06321
Ni	5.23336	7.30730	-1.07184
Ni	3.14329	1.03540	-1.06612
Ni	-5.20707	1.03639	-1.06511
Ni	3.14439	-7.30977	-1.06909
Ni	-5.20965	-7.31251	-1.07064
Ni	1.06330	3.12632	-1.07111
Ni	-7.29708	3.12726	-1.07009
Ni	1.05566	-5.21993	-1.06400
Ni	-7.29860	-5.22437	-1.07255
Ni	-1.03051	-3.13567	-1.06466
Ni	7.31890	-3.13602	-1.07210
Ni	-1.03116	5.22037	-1.06616
Ni	7.32148	5.21722	-1.07256
O	-3.12166	-3.13737	-1.07441
O	5.23291	-3.13606	-1.07455
O	-3.11323	5.21096	-1.05367
O	5.23254	5.21862	-1.07374
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O	-5.21018	-1.04712	-1.07428

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O	1.05022	1.04938	-1.06821
O	-7.29483	1.04243	-1.07370
O	1.05523	-7.31529	-1.06901
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O	-1.03395	3.13093	-1.06807
O	7.32362	3.13095	-1.07557
O	-1.03330	-5.22899	-1.07348
O	7.32152	-5.22466	-1.07579
O	-1.03366	-1.04216	-1.06887
O	7.32202	-1.04676	-1.07638
O	-1.03202	7.29652	-1.05639
O	7.32227	7.30556	-1.07478
O	-3.11574	1.04825	-1.06080
O	5.23512	1.04393	-1.07802
O	-3.11992	-7.31732	-1.06940
O	5.23280	-7.31333	-1.07417
O	3.14065	3.13304	-1.06837
O	-5.20137	3.13057	-1.06160
O	3.14454	-5.22511	-1.07219
O	-5.20914	-5.22631	-1.07498
O	1.05606	-3.13741	-1.07240
O	-7.29768	-3.13625	-1.07610
O	1.05004	5.21534	-1.05995
O	-7.29412	5.21738	-1.07141
Ni	-3.12351	-3.14203	-3.16055
Ni	5.22632	-3.14114	-3.16195
Ni	-3.12494	5.21078	-3.15213
Ni	5.22869	5.21166	-3.16309
Ni	3.13855	-1.05491	-3.15963
Ni	-5.21242	-1.05497	-3.16142
Ni	3.14034	7.30152	-3.16033
Ni	-5.21269	7.29966	-3.15886
Ni	1.05192	1.03051	-3.15640
Ni	-7.30087	1.03301	-3.16306
Ni	1.05202	-7.31652	-3.15830
Ni	-7.30147	-7.31839	-3.16485
Ni	-1.03578	3.11985	-3.15963
Ni	7.31739	3.12208	-3.16392
Ni	-1.03562	-5.22957	-3.15951
Ni	7.31607	-5.22944	-3.16432
Ni	-1.03508	-1.05595	-3.15645

Ni	7.31545	-1.05433	-3.16390
Ni	-1.03604	7.30045	-3.15430
Ni	7.31711	7.30038	-3.16386
Ni	-3.12418	1.03111	-3.15411
Ni	5.22744	1.03274	-3.16384
Ni	-3.12434	-7.31889	-3.15888
Ni	5.22785	-7.31723	-3.16359
Ni	3.14093	3.12123	-3.16075
Ni	-5.21324	3.12117	-3.15680
Ni	3.13884	-5.22817	-3.16013
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Ni	1.05181	-3.14103	-3.15794
Ni	-7.30204	-3.14210	-3.16456
Ni	1.05290	5.21198	-3.15597
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O	3.13987	-3.14166	-3.18352
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O	3.13804	5.21230	-3.18028
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O	1.05019	7.29822	-3.17713
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O	-1.03644	-7.32328	-3.17904
O	7.31766	-7.31929	-3.18507
O	-3.12239	3.12471	-3.17370
O	5.22804	3.12537	-3.18597
O	-3.12395	-5.23237	-3.18467
O	5.22836	-5.23051	-3.18609
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O	5.22872	-1.05211	-3.18704
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O	3.13866	1.03821	-3.18289
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O	3.13937	-7.31952	-3.18350
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O	1.04993	3.12597	-3.17872
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O	7.31871	5.21200	-3.18606
C	0.07967	0.16651	5.91524
O	0.81578	-0.70350	5.38512
O	-0.75894	0.94054	5.34444
H	-0.99030	2.96328	4.53266
C	6.55057	-2.89594	15.08815
C	5.53910	-2.40244	14.27414
C	6.68928	-2.45317	16.37723
C	5.82907	-1.45573	16.87516
C	4.82668	-0.91136	16.02930
C	4.62019	-1.45054	14.72181
H	7.22761	-3.64914	14.71101
C	5.94822	-0.99955	18.20338
C	5.07229	-0.06254	18.68700
C	4.12625	0.50879	17.84632
C	4.03953	0.18558	16.49394
H	5.12733	0.24002	19.72356
C	3.48680	-0.96949	13.93617
C	2.87169	0.25850	14.31398
C	3.19249	0.90011	15.54087
C	2.98480	-1.63580	12.83142
C	1.97995	-1.09188	12.03408
C	1.50041	0.15815	12.30380
C	1.92257	0.87161	13.44962
H	3.37379	-2.60414	12.57083
H	1.60468	-1.64118	11.18164
C	1.42832	2.15354	13.74707
C	1.85166	2.80380	14.87004
C	2.71476	2.17955	15.76789
H	3.01186	2.71161	16.65656
H	0.72161	2.61066	13.06866
H	1.49946	3.80546	15.08545
C	7.74739	-3.02947	17.20776
N	7.80940	-2.51575	18.52098
C	6.97583	-1.53304	19.09870
O	-8.16867	-3.87939	16.83645
O	7.14009	-1.18515	20.25497
O	0.51790	0.76248	11.53196
C	0.45138	0.56023	10.15708
C	1.58986	0.43358	9.37214

C	1.44837	0.28675	8.00828
C	0.18621	0.30980	7.42098
C	-0.94185	0.47476	8.21971
C	-0.81333	0.58122	9.58883
H	2.56859	0.44161	9.83551
H	2.32074	0.17254	7.37444
H	-1.92496	0.49848	7.76245
H	-1.67861	0.68907	10.23295
O	5.42512	-2.92060	12.98927
C	6.59315	-3.22491	12.27810
C	7.64011	-2.32750	12.19760
C	-7.95759	-2.65041	11.43702
C	-7.87349	-3.85204	10.74250
C	7.75401	-4.72873	10.84425
C	6.64367	-4.43129	11.60814
H	7.77986	-5.67884	10.32389
H	5.81329	-5.12096	11.69190
H	-7.14752	-1.93575	11.39048
H	7.58452	-1.38451	12.72688
C	-6.65772	-4.23913	9.89320
C	-5.57996	-3.15048	9.89298
H	-4.73575	-3.46302	9.27711
H	-5.19692	-2.95395	10.89494
H	-5.95127	-2.20971	9.48402
C	-7.10632	-4.47113	8.44090
H	-7.84123	-5.27211	8.36432
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C	-6.03881	-5.53010	10.45450
H	-6.74188	-6.36240	10.42987
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H	-5.16181	-5.82266	9.87422
O	3.19396	1.36925	18.40816
C	3.63231	2.47925	19.13849
C	2.78434	2.96277	20.11928
C	3.14972	4.08829	20.82947
C	4.35328	4.75559	20.59118
C	5.17515	4.24669	19.59336
C	4.82512	3.12006	18.86231
H	1.85319	2.44579	20.31451
H	5.48041	2.73572	18.08999
H	6.11666	4.72730	19.36406
H	2.47704	4.45056	21.59854

C	4.71697	5.99234	21.42530
C	6.07070	6.58669	21.02321
H	6.88468	5.87156	21.15986
H	6.29480	7.45900	21.64382
H	6.07960	6.91795	19.98098
C	4.78786	5.59516	22.91287
H	5.53669	4.81759	23.07691
H	3.83434	5.21156	23.27608
H	5.05432	6.45712	23.53147
C	3.63995	7.07441	21.23167
H	3.56255	7.36975	20.18235
H	3.87828	7.96780	21.81588
H	2.65644	6.72743	21.54848
N	-7.88866	-3.03266	19.34483
C	-6.65386	-2.35418	19.31827
C	-5.61261	-2.91241	20.20494
C	-5.88998	-4.04201	21.00404
C	-7.15102	-4.67583	20.98497
C	-8.22815	-4.16511	20.11262
O	-6.48528	-1.38315	18.60807
O	7.37408	-4.66414	20.04119
C	-4.37521	-2.31453	20.24358
C	-3.37352	-2.81829	21.07541
C	-3.61442	-3.91650	21.86552
C	-4.87638	-4.55232	21.84809
H	-4.19610	-1.44908	19.61922
H	-2.39616	-2.35383	21.11223
C	-5.15675	-5.68176	22.64928
C	-6.39514	-6.27659	22.61076
C	-7.39460	-5.77280	21.77627
H	-6.57839	-7.13947	23.23800
H	8.33471	-6.23471	21.73841
C	-2.54450	-4.43685	22.74233
N	-2.88837	-5.55235	23.50560
C	-4.10860	-6.22804	23.53641
O	-1.42702	-3.95207	22.81984
O	-4.26197	-7.19977	24.25883
H	-2.16449	-5.91535	24.11114