

Supporting Information

Electronic Coupling in Metallophthalocyanine- Transition Metal Dichalcogenide Mixed- Dimensional Heterojunctions

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Table S1. E_{REL} (standard deviation) for each phthalocyanine and layer number with 633 nm excitation laser

	1L	2L	3L	Bulk
CoPc	25.8 (3.2)	48.2 (10.2)	14.8 (2.1)	1.7
NiPc	23.4 (3.6)	26.5 (7.2)	14.1 (1.3)	0.5
CuPc	9.2 (0.9)	6 (0.8)	5.1 (1.0)	*
ZnPc	4.9 (0.7)	4.9 (1.7)	2.1 (0.3)	0.6
H ₂ Pc	*	*	*	*

*Signal too weak to measure

Table S2. E_{REL} (standard deviation) for each phthalocyanine and layer number with 532 nm excitation laser

	1L	2L	3L	Bulk
CoPc	2.5 (0.3)	2.1 (0.1)	1.7 (0.2)	*
NiPc	2.9(0.2)	1.8 (0.2)	2.2(0.1)	*
CuPc	3.9 (0.1)	2.7 (0.2)	1.6 (0.1)	*
ZnPc	0.6 (0.1)	0.5 (0.2)	*	*
H ₂ Pc	1.6 (0.4)	1.4 (0.6)	0.9 (0.3)	*

*Signal too weak to measure

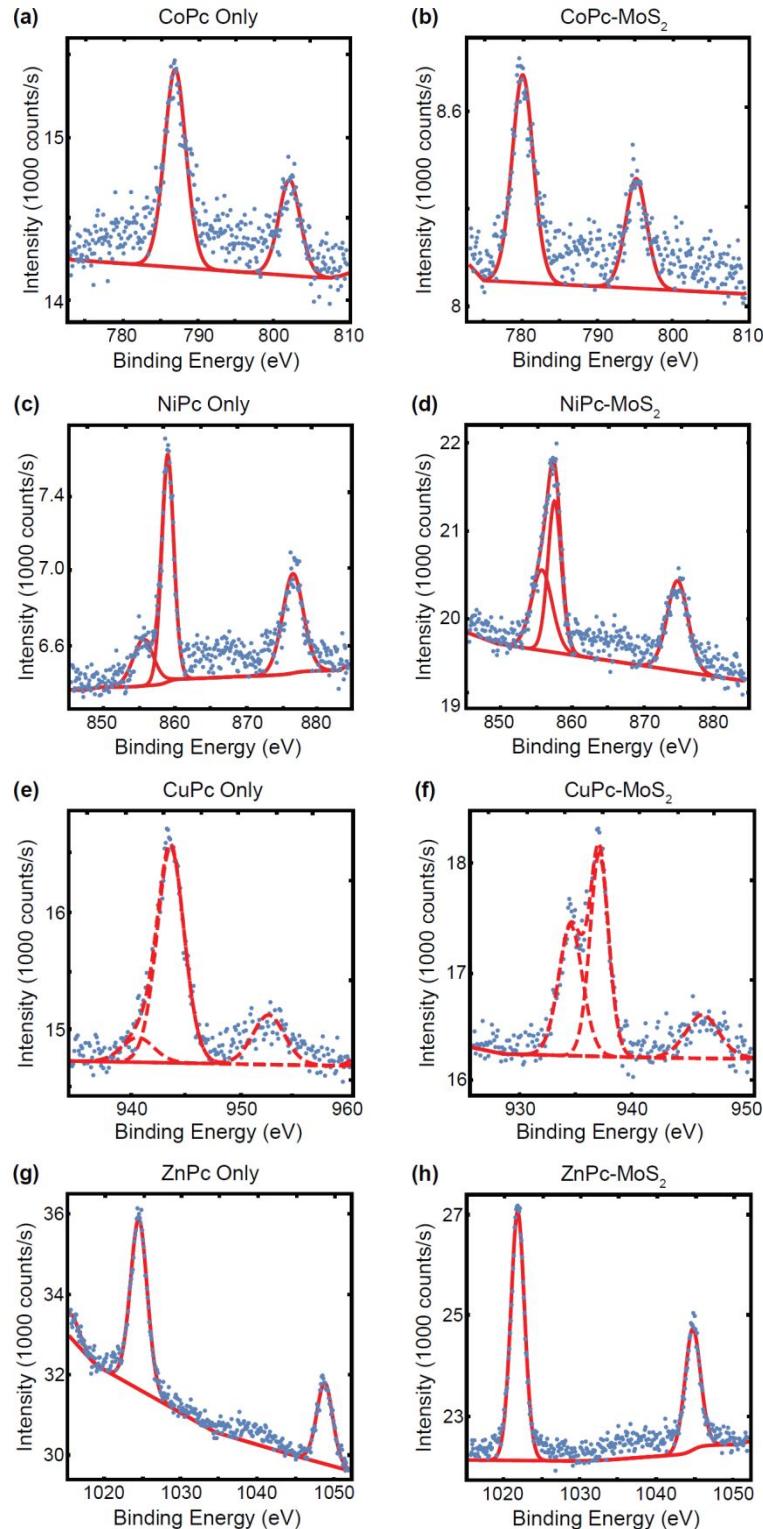


Figure S1. X-ray photoelectron spectra (XPS) of MPC metal core electrons (a, b: Co 2p; c, d: Ni 2p; e, f: Cu 2p; g, h: Zn 2p) with identical film thickness on sapphire or CVD MoS₂ – sapphire substrates. Peak integrations indicate similar amounts of MPC is deposited on sapphire *versus* MoS₂. Due to the insulating substrate and long collection times, significant charging effects occur despite the use of a charge

compensation gun. This causes large shifts in the peak positions, meaning subtle changes in chemical state on sapphire *versus* MoS₂ are not observable. The charge compensation also causes reduction of the Cu²⁺ species over time, which yields the different peak structure in the Cu 2p spectra on sapphire *versus* MoS₂.

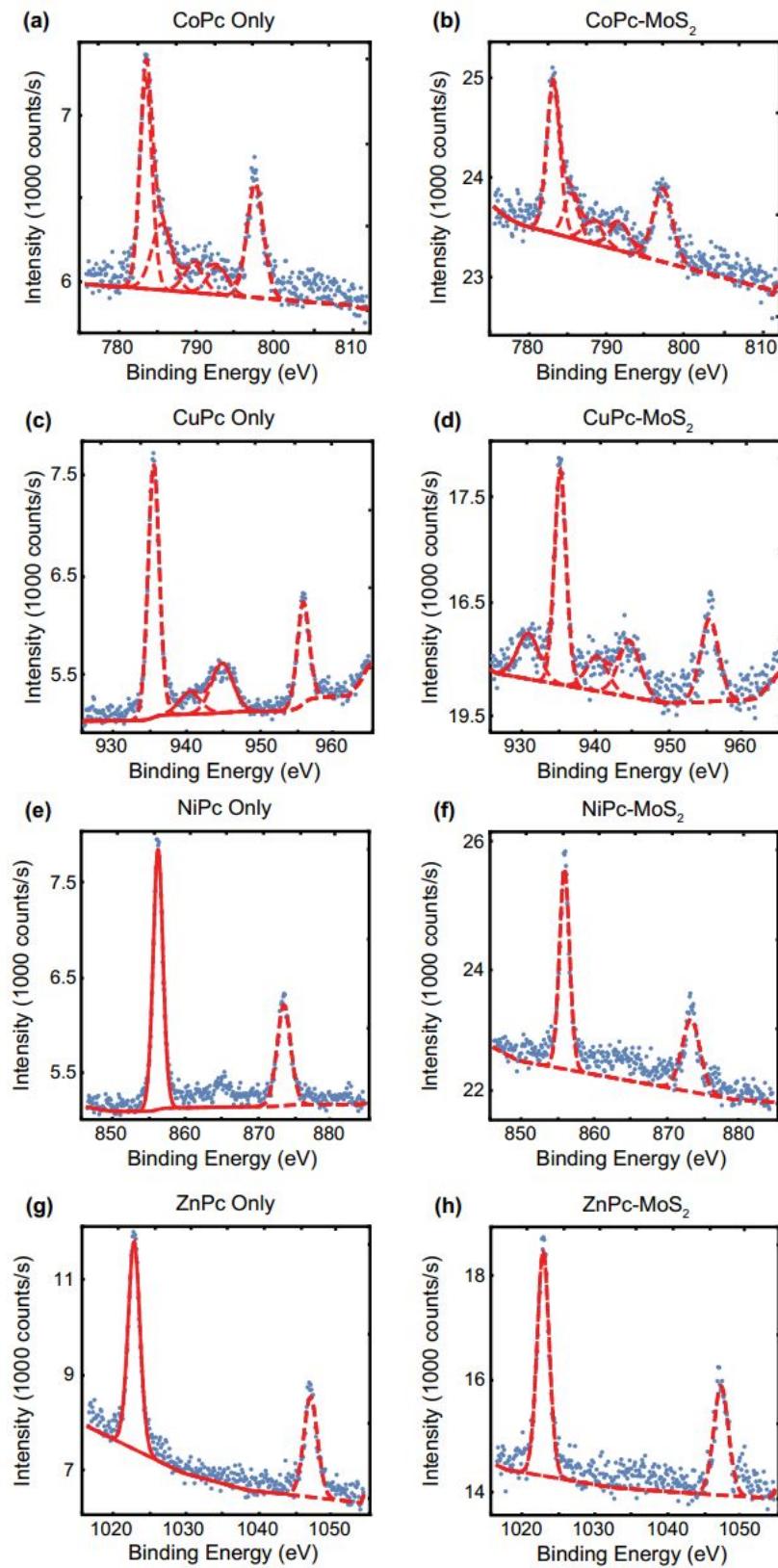


Figure S2. X-ray photoelectron spectra (XPS) of MPC metal core electrons (a, b: Co 2p; c, d: Ni 2p; e, f: Cu 2p; g, h: Zn 2p) with identical film thickness deposited on native silicon oxide and bulk MoS₂ – conductive carbon tape substrates. Deposition on conducting substrates reduced charging effects and allowed more accurate quantification. Peak integrations indicate similar amounts of MPC is deposited on oxide *versus* MoS₂, confirming similar behavior on silicon oxide as with sapphire. The additional Cu peak near 930 eV in (d) is a result of partial reduction of the Cu²⁺ by the charge compensating flood gun.

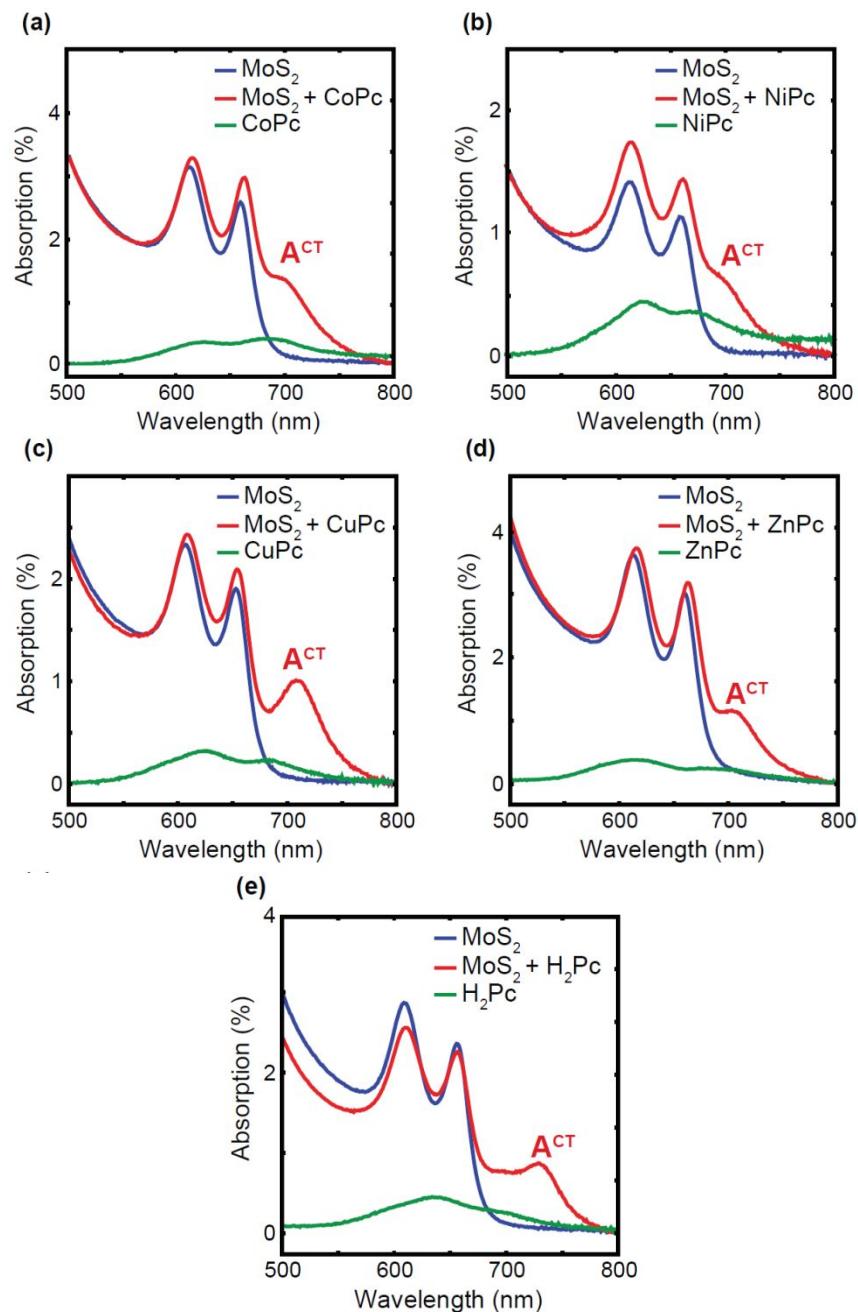


Figure S3. Absorption spectra of monolayer chemical vapor deposition grown MoS₂, 0.4 nm of Pc, and MoS₂ with 0.4 nm Pc deposited. The emergent charge-transfer absorption is labeled A^{CT}. All spectra were taken on sapphire substrates.

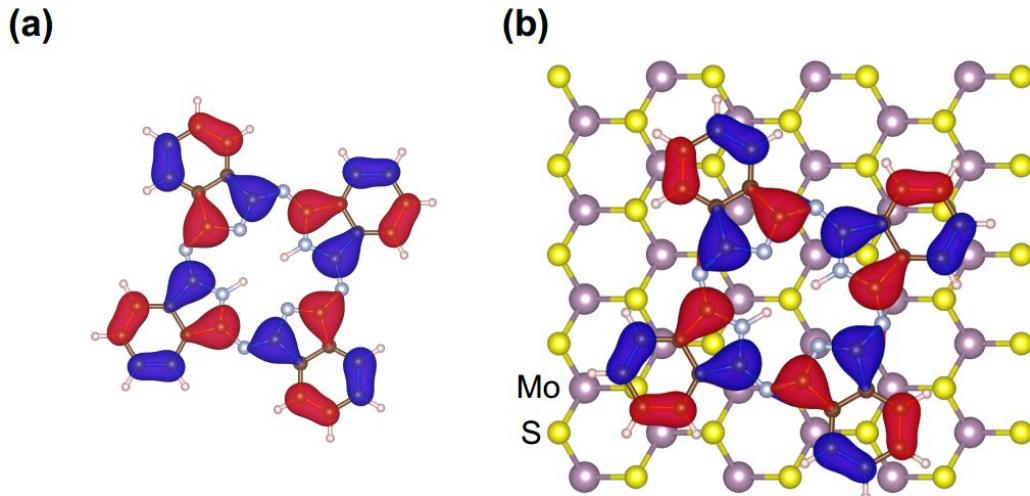
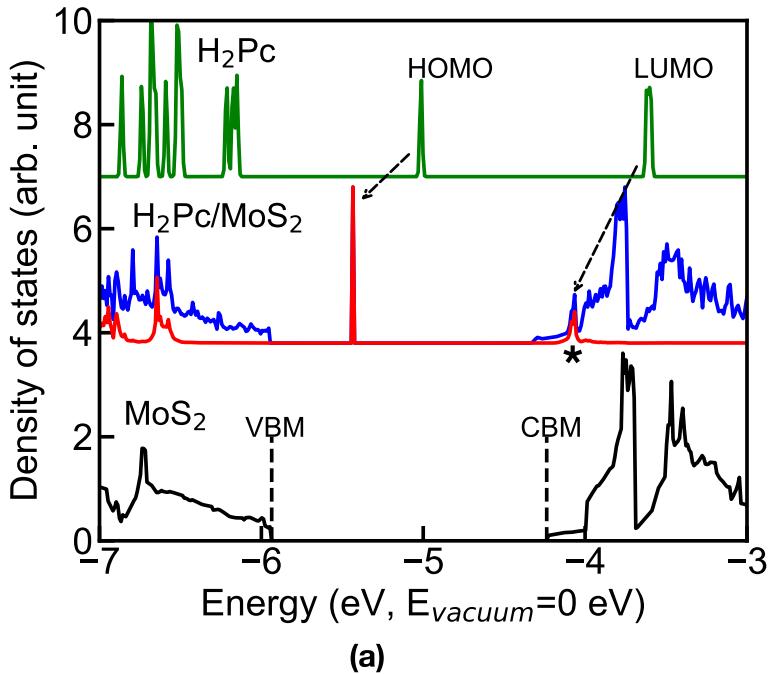


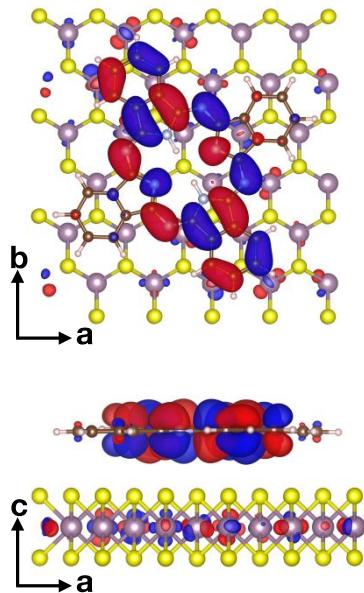
Figure S4. Charge densities from calculations: (a) HOMO of H₂Pc; (b) HOMO of H₂Pc on MoS₂

Based on our DFT calculations, we expect the LUMO of the MPc to have (1) an out-of-plane e_g (d_{xz} , d_{yz}) character, and (2) be at resonance with the conduction band of MoS₂ of d_{xy} and $d_{x^2-y^2}$ character (near the conduction band minimum) and (d_{xz} , d_{yz}) at higher energies, resulting in mixing between the LUMO and MoS₂ orbitals.

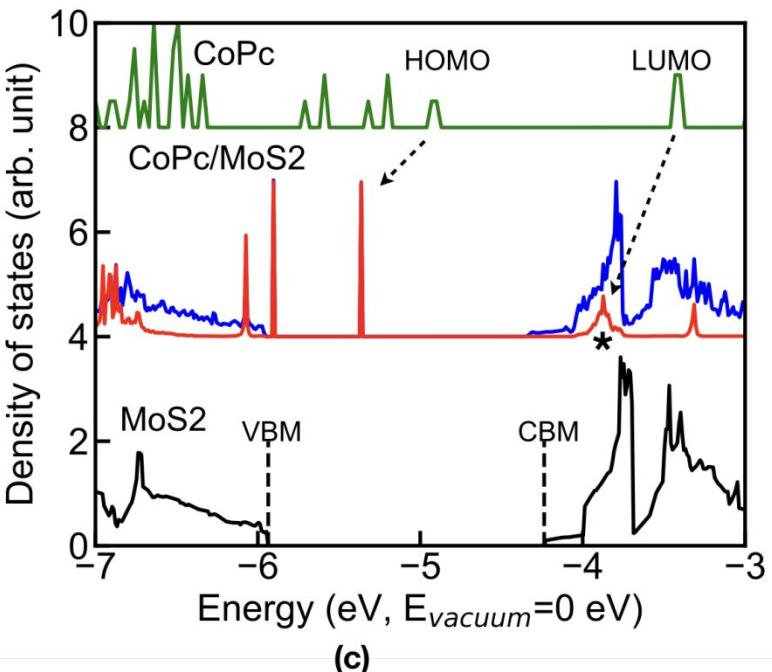
In Figure S4, we plot the projected Density of States (pDOS) for H₂Pc - MoS₂ and CoPc - MoS₂ computed using the PBE functional in Figure S4 of the SI (it is important to note the semi-local PBE functional is not expected to give a quantitative picture in the case of MPc). In contrast with other the weakly-coupled molecular orbitals, the LUMO of CoPc is shown to have >0.1V spectral broadening. This hybridization can also be observed in the wavefunction of the combined CoPc - MoS₂ at the energy corresponding to the maximum of the LUMO projection: As shown in Figure S4, the eigenstate of the combined-system Hamiltonian has significant MoS₂ character.



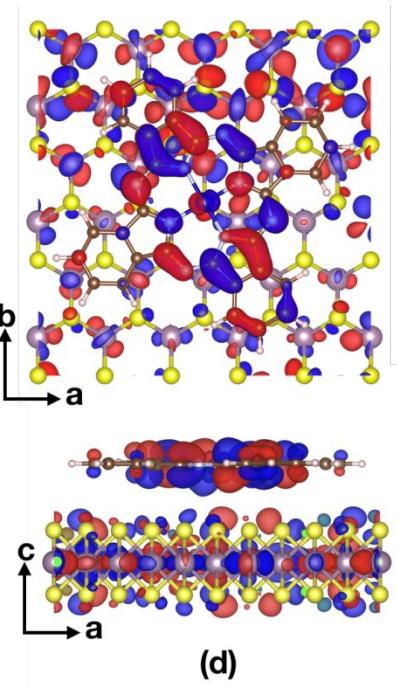
(a)



(b)



(c)



(d)

Figure S5. Density of states (DOS) for isolated MPc (green) and 1ML MoS₂ (black), and for MPc- MoS₂ (blue) with projected density of states of MPc in MPc- MoS₂ heterojunctions in red for H₂Pc and CoPc in (a) and (c), respectively. The HOMO of MPc- MoS₂ is located purely on MPc, as shown in (c). The wavefunction corresponding at the energy of the LUMO of Pc, as shown by * in (a) and (c) are shown in (b) and (d) respectively for H₂Pc - MoS₂ and CoPc – MoS₂. Results here are from calculations with PBE functionals.

As expected from the gas-phase electronic band-offsets, all molecules are donating electrons to MoS₂, in agreement with the downshift of the HOMO. As can be seen in Figure S5, the electronic density changes upon absorption for all molecules are very similar, with corresponding changes in HOMO energies within 0.1 eV of each other (please note that all these calculations are done using a semilocal functional which does not quantitatively describe the d-orbitals of MPc). This further reinforces our claim that the ground-state charge transfer is weakly impacted by the metal center (in agreement with the weak changes in the onset of optical absorption), in contrast with the excited-state charge transfer that involves the d-orbitals of the metal center (non-frontier orbitals).

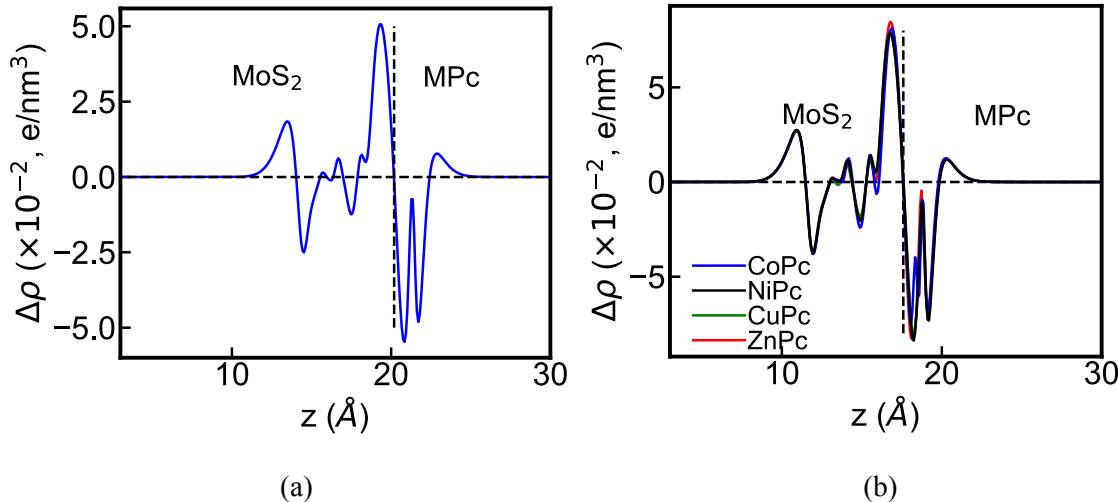


Figure S6. Charge density change $\Delta\rho$ upon adsorption of H₂Pc (a) and transition metal MPc (b) on MoS₂, for $\Delta\rho = \rho[\text{MPc-MoS}_2] - \rho[\text{MPc}] - \rho[\text{MoS}_2]$, where the three terms on the right represent the charge density of MPc- MoS₂, isolated MPc and MoS₂, respectively. The vertical dashed line depicts the location of the interface, with MoS₂ on the left and MPc on the right.

molecule	$\Delta E(\text{eV})$	$P_{\text{tot}}(\text{D}/\text{nm}^2)$	$P_{\text{ind}}(\text{D}/\text{nm}^2)$	$\Delta E^*(\text{eV})$	$E_{\text{binding}}(\text{eV/molecule})$
H2Pc	0.4363	0.5102	0.5599	0.1939	1.5960
CoPc	0.4557	0.4346	0.4671	0.1652	1.9530
NiPc	0.4416	0.5140	0.5745	0.1953	1.5793
CuPc	0.3750	0.4985	0.5615	0.1894	1.6628
ZnPc	0.3845	0.3860	0.5423	0.1467	1.5945

Table S3. Change in energy between the gas phase Pc HOMO and the Pc-MoS₂ HOMO and interface dipole: $\Delta E(\text{eV})$ refers to the observed shift in HOMO energy between the gas phase Pc and the adsorbed Pc computed in DFT-PBE. P_{tot} is the normal component of the areal dipole of the heterojunction; P_{ind} is the induced areal dipole (computed from the change in electronic density upon absorption). ΔE^* is the resulting far-field potential change computed using a classical parallel plate capacitor model. E_{binding} is the binding energy of Pc-MoS₂.

Moreover, we assess the role of the interface dipole in the energy shift of the molecular level using a classical parallel-plate capacitor model (assuming a dielectric function of 1, and approximating the HOMO by a point charge in the far field). As shown in table S2, the resulting dipole-induced energy shifts, while commensurate with the DFT calculations, only accounts for ~36-51% (depending on the molecule) of the observed energy shifts, implying higher moments of the density play a significant role in the observed shift in electronic energies.

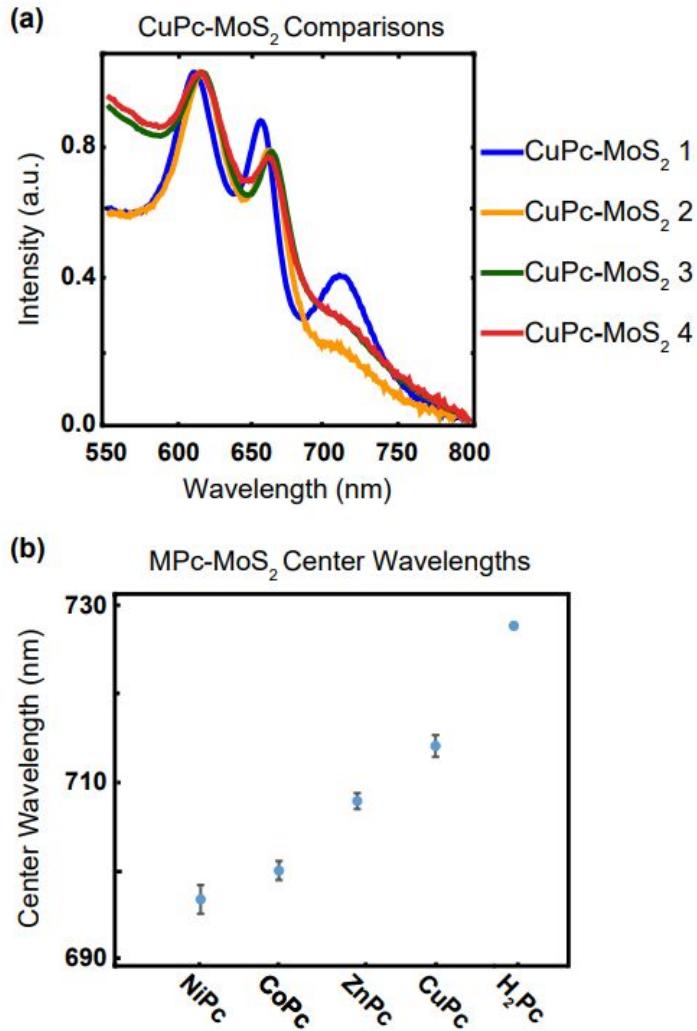


Figure S7. (a) Reproducibility on CuPc absorption show consistent CT-peak position but variable intensity, we correlate the intensity rather than the peak position to variable underlying MoS₂ morphologies. (b) Mpc absorptions CT-peak wavelength with error. Wavelength was extracted by Lorentzian fits and errors from fit uncertainty except in CuPc, which was found from (a) reproducibility runs.

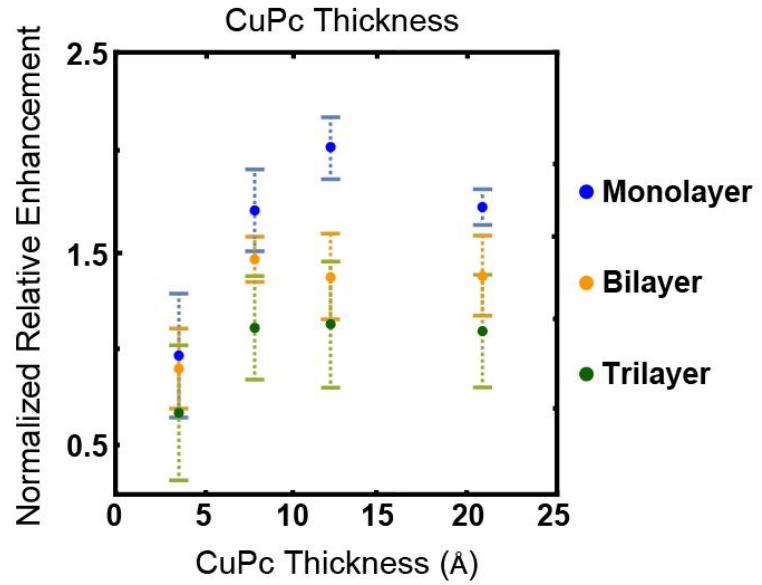


Figure S8. Thickness dependent relative enhancement factor for CuPc-MoS₂ heterojunction. Relative enhancement increases with CuPc film thickness up to ~12 Å before levelling off. This is consistent with the Raman enhancement being a first layer effect that exponentially decreases with distance

Coordinates of gas phase MPc (M=H₂, Co,Ni,Cu,Zn) molecules optimized from PBE and HSE, respectively, and that of MPc-MoS₂ heterostructure optimized from PBE functional.

H₂Pc from HSE

C	15.30724000	6.76930700	16.50454000
C	16.32774000	6.78191100	15.55710000
C	15.66084000	6.81314700	14.26230000
C	14.06522000	6.79246000	15.74378000
C	11.74134000	6.80451600	15.71674000
C	10.19486000	6.84136900	14.05638000
C	10.43848000	6.80794100	16.33710000
C	9.48298000	6.83013500	15.31166000
C	10.33916000	6.88562000	11.73770000
C	10.69302000	6.92987100	9.49546000
C	9.67226000	6.91699300	10.44290000
C	14.25866000	6.89452500	10.28326000
C	15.80514000	6.85712400	11.94362000
C	16.51702000	6.86808400	10.68834000
C	15.56152000	6.89068900	9.66290000
C	11.93478000	6.90658100	10.25622000
C	15.58414000	6.73930400	17.85888000
C	17.65790000	6.76423800	15.93306000
C	10.05706000	6.79670700	17.67064000
C	8.12552000	6.84123200	15.59922000
C	17.87448000	6.85643900	10.40052000
C	15.94294000	6.90206000	8.32936000
C	7.75112000	6.82945000	16.92782000
C	8.70558000	6.80753000	17.95170000
C	8.34210000	6.93480300	10.06694000

C	8.06078000	6.96508000	8.71000000
C	9.08284000	6.97713600	7.76048000
C	10.41586000	6.96014800	8.14112000
C	16.91716000	6.72259000	18.23926000
C	17.93948000	6.73437200	17.29000000
C	17.29442000	6.89082600	8.04804000
C	18.24888000	6.86835800	9.07192000
H	12.26082000	6.82890200	13.68146000
H	13.73918000	6.87000200	12.31854000
H	14.78698000	6.73026200	18.58870000
H	18.44440000	6.77328000	15.19154000
H	10.80066000	6.78040400	18.45454000
H	7.39492000	6.85959000	14.80336000
H	18.60508000	6.83753300	11.19638000
H	6.70150000	6.83821800	17.18730000
H	8.37356000	6.79931000	18.98078000
H	7.55560000	6.92548700	10.80820000
H	7.03144000	6.97932800	8.37746000
H	8.82674000	7.00001500	6.70982000
H	11.21302000	6.96932700	7.41130000
H	17.17326000	6.69984800	19.29018000
H	18.96856000	6.72012400	17.62254000
H	19.29850000	6.85904200	8.81244000
H	15.19934000	6.91877400	7.54546000
H	17.62644000	6.89904600	7.01896000
N	14.31534000	6.81821600	14.41336000
N	12.88586000	6.78752800	16.34698000
N	11.52320000	6.82369600	14.36968000
N	9.64990000	6.86712500	12.86922000
N	11.68466000	6.88055100	11.58664000

N	14.47680000	6.87520800	11.63006000
N	16.35010000	6.83123100	13.13078000
N	13.111414000	6.91165000	9.65276000

CoPc from HSE

C	15.29476000	6.76862200	16.47854000
C	16.31188000	6.77054000	15.52954000
C	15.66240000	6.79848800	14.23890000
C	14.05170000	6.79465200	15.74196000
C	11.76006000	6.82150400	15.66318000
C	10.25778000	6.86644000	14.05248000
C	10.46864000	6.82492900	16.31240000
C	9.52016000	6.85356200	15.29528000
C	10.33760000	6.90192300	11.76110000
C	10.70524000	6.93151500	9.52146000
C	9.68812000	6.92973400	10.47046000
C	14.23994000	6.87877000	10.33682000
C	15.74222000	6.83410800	11.94752000
C	16.47958000	6.84698600	10.70472000
C	15.53136000	6.87548200	9.68760000
C	11.94830000	6.90548500	10.25804000
C	15.57530000	6.74464700	17.83522000
C	17.64620000	6.74766100	15.90238000
C	10.09424000	6.80588600	17.64620000
C	8.16322000	6.86328900	15.57452000
C	17.83678000	6.83753300	10.42548000
C	15.90576000	6.89438800	8.35380000
C	7.78674000	6.84301300	16.90494000
C	8.74042000	6.81492800	17.92752000

C	8.35380000	6.95261300	10.09762000
C	8.07170000	6.97631400	8.74432000
C	9.09376000	6.97741000	7.79012000
C	10.42470000	6.95549000	8.16478000
C	16.90624000	6.72259000	18.20988000
C	17.92830000	6.72382300	17.25568000
C	17.25958000	6.88562000	8.07248000
C	18.21326000	6.85780900	9.09506000
Co	13.00000000	6.85013700	13.00000000
H	14.77918000	6.74368800	18.56608000
H	18.42958000	6.74875700	15.15774000
H	10.83758000	6.78478800	18.43036000
H	7.43366000	6.88534600	14.77762000
H	18.56634000	6.81547600	11.22238000
H	6.73686000	6.84931500	17.16442000
H	8.40814000	6.80054300	18.95686000
H	7.57042000	6.95165400	10.84226000
H	7.04210000	6.99426100	8.41308000
H	8.83350000	6.99576800	6.74050000
H	11.22082000	6.95631200	7.43392000
H	17.16650000	6.70409500	19.25950000
H	18.95790000	6.70587600	17.58692000
H	19.26314000	6.85164400	8.83558000
H	15.16242000	6.91548600	7.56964000
H	17.59186000	6.90000500	7.04314000
N	14.30468000	6.81232500	14.39854000
N	12.88404000	6.79807700	16.33476000
N	11.60094000	6.84616400	14.30546000
N	9.66550000	6.89247000	12.88508000
N	11.69532000	6.88794900	11.60172000

N	14.39906000	6.85424700	11.69454000
N	16.33450000	6.80807800	13.11492000
N	13.111596000	6.90206000	9.66524000

NiPc from HSE

C	15.30594000	6.77410200	16.51156000
C	16.32956000	6.77944500	15.56152000
C	15.68502000	6.80725600	14.26282000
C	14.05924000	6.79670700	15.77160000
C	11.73666000	6.81602400	15.68502000
C	10.22788000	6.85548000	14.05976000
C	10.43822000	6.81753100	16.32982000
C	9.48792000	6.84246500	15.30646000
C	10.31498000	6.89301800	11.73718000
C	10.69406000	6.92603500	9.48844000
C	9.67044000	6.92069200	10.43848000
C	14.26334000	6.88425000	10.31498000
C	15.77212000	6.84493100	11.94024000
C	16.51208000	6.85808300	10.69354000
C	15.56178000	6.88274300	9.67018000
C	11.94076000	6.90356700	10.22840000
C	15.58544000	6.75094900	17.86772000
C	17.66102000	6.75930600	15.94242000
C	10.05784000	6.80246100	17.66128000
C	8.13176000	6.85232900	15.58726000
C	17.86824000	6.84835600	10.41274000
C	15.94216000	6.89781300	8.33872000
C	7.75242000	6.83712200	16.91742000
C	8.70350000	6.81273600	17.94156000

C	8.33898000	6.94083100	10.05758000
C	8.06000000	6.96466900	8.70298000
C	9.08440000	6.96795700	7.75242000
C	10.41456000	6.94918800	8.13228000
C	16.91560000	6.73218000	18.24758000
C	17.94000000	6.73546800	17.29702000
C	17.29650000	6.88781200	8.05870000
C	18.24758000	6.86356300	9.08258000
H	14.78750000	6.74875700	18.59650000
H	18.44778000	6.76218300	15.20142000
H	10.79936000	6.78396600	18.44752000
H	7.40246000	6.87178300	14.78984000
H	18.59754000	6.82890200	11.21016000
H	6.70176000	6.84506800	17.17378000
H	8.37018000	6.80246100	18.97038000
H	7.55222000	6.93795400	10.79858000
H	7.03118000	6.98042400	8.36966000
H	8.82882000	6.98508200	6.70176000
H	11.21250000	6.95138000	7.40350000
H	17.17118000	6.71505500	19.29824000
H	18.96882000	6.71957600	17.63034000
H	19.29824000	6.85561700	8.82622000
H	15.20064000	6.91630800	7.55248000
H	17.62982000	6.89808700	7.02962000
N	14.33484000	6.81643500	14.43832000
N	12.87494000	6.79602200	16.34594000
N	11.56142000	6.83945100	14.33484000
N	9.65380000	6.87959200	12.87546000
N	11.66516000	6.88383900	11.56168000
N	14.43858000	6.86082300	11.66516000

N	16.34646000	6.82068200	13.12454000
N	13.12506000	6.90425200	9.65406000
Ni	13.00000000	6.85013700	13.00000000

CuPc from HSE

C	15.30542000	6.77369100	16.49752000
C	16.32592000	6.77917100	15.54722000
C	15.67852000	6.80616000	14.25164000
C	14.05924000	6.79725500	15.75990000
C	11.74784000	6.82027100	15.67826000
C	10.23984000	6.85986400	14.05950000
C	10.45226000	6.82232600	16.32592000
C	9.50170000	6.84726000	15.30568000
C	10.32148000	6.89630600	11.74810000
C	10.69458000	6.92822700	9.50222000
C	9.67382000	6.92261000	10.45278000
C	14.25216000	6.88342800	10.32148000
C	15.76016000	6.84356100	11.94050000
C	16.49804000	6.85643900	10.69432000
C	15.54774000	6.88164700	9.67382000
C	11.94050000	6.90534800	10.24010000
C	15.58648000	6.74916800	17.85368000
C	17.65894000	6.76053900	15.92396000
C	10.07500000	6.80479000	17.65868000
C	8.14554000	6.85589100	15.58674000
C	17.85446000	6.84808200	10.41300000
C	15.92474000	6.89932000	8.34106000
C	7.76854000	6.83862900	16.91716000
C	8.72118000	6.81328400	17.94000000

C	8.34106000	6.94069400	10.07604000
C	8.06000000	6.96466900	8.72222000
C	9.08284000	6.97042300	7.76958000
C	10.41326000	6.95220200	8.14606000
C	16.91690000	6.73039900	18.23042000
C	17.94000000	6.73587900	17.27778000
C	17.27882000	6.89110000	8.06000000
C	18.23146000	6.86561800	9.08284000
Cu	13.00000000	6.85164400	13.00000000
H	14.78958000	6.74505800	18.58350000
H	18.44362000	6.76492300	15.18114000
H	10.81782000	6.78519900	18.44336000
H	7.41572000	6.87534500	14.79010000
H	18.58428000	6.82862800	11.20990000
H	6.71840000	6.84465700	17.17560000
H	8.38864000	6.80013200	18.96908000
H	7.55612000	6.93617300	10.81886000
H	7.03092000	6.97919100	8.38994000
H	8.82466000	6.98919200	6.71944000
H	11.21016000	6.95644900	7.41624000
H	17.17508000	6.71094500	19.28030000
H	18.96908000	6.72080900	17.61006000
H	19.28160000	6.85986400	8.82414000
H	15.18218000	6.91877400	7.55638000
H	17.61110000	6.90425200	7.03092000
N	14.32730000	6.81602400	14.42454000
N	12.88144000	6.79944700	16.34256000
N	11.57520000	6.84273900	14.32730000
N	9.65718000	6.88425000	12.88196000
N	11.67244000	6.88671600	11.57546000

N	14.42480000	6.86068600	11.67244000
N	16.34282000	6.81862700	13.11804000
N	13.11830000	6.90370400	9.65718000

ZnPc from HSE

C	15.31998000	6.77259500	16.51884000
C	16.34412000	6.77848600	15.56568000
C	15.69828000	6.80520100	14.26594000
C	14.06964000	6.79561100	15.78174000
C	11.73354000	6.81780500	15.69828000
C	10.21774000	6.85767200	14.07016000
C	10.43354000	6.81958600	16.34438000
C	9.48064000	6.84479400	15.32050000
C	10.30172000	6.89493600	11.73406000
C	10.68002000	6.92767900	9.48116000
C	9.65588000	6.92165100	10.43432000
C	14.26646000	6.88246900	10.30172000
C	15.78226000	6.84260200	11.92984000
C	16.51936000	6.85561700	10.67950000
C	15.56646000	6.88068800	9.65562000
C	11.93036000	6.90466300	10.21826000
C	15.60416000	6.74834600	17.87422000
C	17.67584000	6.75999100	15.94554000
C	10.05342000	6.80218700	17.67584000
C	8.12500000	6.85356200	15.60494000
C	17.87500000	6.84684900	10.39532000
C	15.94658000	6.89808700	8.32416000
C	7.74722000	6.83616300	16.93536000
C	8.69908000	6.81068100	17.95768000

C	8.32416000	6.94014600	10.05420000
C	8.04258000	6.96439500	8.70038000
C	9.06516000	6.97014900	7.74826000
C	10.39584000	6.95179100	8.12578000
C	16.93484000	6.72985100	18.25174000
C	17.95742000	6.73560500	17.29962000
C	17.30092000	6.88973000	8.04232000
C	18.25278000	6.86438500	9.06464000
H	14.80778000	6.74396200	18.60482000
H	18.46130000	6.76464900	15.20324000
H	10.79546000	6.78287000	18.46130000
H	7.39440000	6.87342700	14.80856000
H	18.60560000	6.82698400	11.19144000
H	6.69682000	6.84232800	17.19328000
H	8.36680000	6.79752900	18.98702000
H	7.53870000	6.93548800	10.79650000
H	7.01350000	6.97946500	8.36810000
H	8.80750000	6.98946600	6.69812000
H	11.19222000	6.95617500	7.39518000
H	17.19250000	6.71067100	19.30188000
H	18.98676000	6.72053500	17.63190000
H	19.30318000	6.85822000	8.80672000
H	15.20454000	6.91754100	7.53870000
H	17.63320000	6.90288200	7.01298000
N	14.35070000	6.81424300	14.45132000
N	12.87962000	6.79725500	16.35114000
N	11.54842000	6.84068400	14.35096000
N	9.64886000	6.88233200	12.88014000
N	11.64930000	6.88589400	11.54868000
N	14.45158000	6.85959000	11.64904000

N	16.35114000	6.81794200	13.11986000
N	13.12038000	6.90301900	9.64912000
Zn	13.00000000	6.85013700	13.00000000

H₂Pc from PBE

C	15.32544000	6.76930700	16.53158000
C	16.35530000	6.77821200	15.57660000
C	15.68710000	6.80848900	14.27374000
C	14.07588000	6.79109000	15.76848000
C	11.73224000	6.80259800	15.73988000
C	10.17094000	6.84301300	14.06392000
C	10.42158000	6.80794100	16.36180000
C	9.45776000	6.83260100	15.32726000
C	10.31290000	6.89014100	11.72600000
C	10.67456000	6.92973400	9.46816000
C	9.64470000	6.92069200	10.42340000
C	14.26776000	6.89630600	10.25986000
C	15.82906000	6.85575400	11.93608000
C	16.54224000	6.86602900	10.67274000
C	15.57842000	6.89068900	9.63820000
C	11.92412000	6.90767700	10.23152000
C	15.60624000	6.74464700	17.89424000
C	17.69300000	6.76012800	15.95880000
C	10.03574000	6.79615900	17.70236000
C	8.09354000	6.84589000	15.61794000
C	17.90646000	6.85232900	10.38206000
C	15.96452000	6.90206000	8.29764000
C	7.71472000	6.83451900	16.95616000
C	8.67412000	6.80999600	17.98576000

C	8.30700000	6.93891300	10.04120000
C	8.02334000	6.96521700	8.67438000
C	9.05216000	6.97206700	7.72044000
C	10.39402000	6.95466800	8.10576000
C	16.94784000	6.72779600	18.27956000
C	17.97666000	6.73450900	17.32536000
C	17.32588000	6.88794900	8.01424000
C	18.28528000	6.86342600	9.04384000
H	12.25718000	6.82698400	13.68406000
H	13.74282000	6.87192000	12.31594000
H	14.80310000	6.73957800	18.62848000
H	18.48574000	6.76601900	15.21312000
H	10.78402000	6.77684200	18.49172000
H	7.35826000	6.86452200	14.81610000
H	18.64174000	6.83356000	11.18364000
H	6.65756000	6.84452000	17.21590000
H	8.34054000	6.80191300	19.02212000
H	7.51426000	6.93261100	10.78662000
H	6.98724000	6.98028700	8.34002000
H	8.79684000	6.99124700	6.66198000
H	11.19716000	6.95960000	7.37152000
H	17.20342000	6.70902700	19.33802000
H	19.01276000	6.71985000	17.65972000
H	19.34244000	6.85301400	8.78410000
H	15.21598000	6.92137700	7.50802000
H	17.65946000	6.89575800	6.97788000
N	14.32730000	6.81465400	14.42428000
N	12.88612000	6.78725400	16.37584000
N	11.51228000	6.82081900	14.37956000
N	9.61948000	6.87260500	12.86740000

N	11.67270000	6.88397600	11.57572000
N	14.48772000	6.87835900	11.62044000
N	16.38052000	6.82602500	13.13234000
N	13.11388000	6.91165000	9.62416000

CoPc from PBE

C	15.30412000	6.77245800	16.50324000
C	16.33008000	6.77807500	15.54748000
C	15.68346000	6.80451600	14.24852000
C	14.05430000	6.79574800	15.76588000
C	11.74966000	6.81862700	15.68476000
C	10.23308000	6.85959000	14.05586000
C	10.45044000	6.82081900	16.33164000
C	9.49494000	6.84671200	15.30516000
C	10.31654000	6.89562100	11.75148000
C	10.69588000	6.92767900	9.49702000
C	9.66992000	6.92192500	10.45252000
C	14.25034000	6.88178400	10.31524000
C	15.76692000	6.84082100	11.94414000
C	16.50506000	6.85369900	10.69484000
C	15.54956000	6.87959200	9.66836000
C	11.94570000	6.90438900	10.23412000
C	15.58622000	6.74807200	17.86798000
C	17.67168000	6.75999100	15.92552000
C	10.07110000	6.80259800	17.67272000
C	8.12994000	6.85534300	15.58726000
C	17.87006000	6.84534200	10.41274000
C	15.92890000	6.89808700	8.32728000
C	7.74930000	6.83698500	16.92704000

C	8.70740000	6.81095500	17.95638000
C	8.32832000	6.94014600	10.07448000
C	8.04466000	6.96425800	8.71078000
C	9.07374000	6.97014900	7.75242000
C	10.41378000	6.95206500	8.13202000
C	16.92626000	6.72985100	18.24758000
C	17.95534000	6.73574200	17.28922000
C	17.29260000	6.88986700	8.04362000
C	18.25070000	6.86383700	9.07296000
Co	13.00000000	6.85013700	13.00000000
H	14.78360000	6.74382500	18.60222000
H	18.46104000	6.76478600	15.17698000
H	10.81912000	6.78245900	18.46260000
H	7.39570000	6.87520800	14.78464000
H	18.60430000	6.82547700	11.21536000
H	6.69162000	6.84273900	17.18626000
H	8.37330000	6.79698100	18.99248000
H	7.53896000	6.93535100	10.82302000
H	7.00830000	6.97891700	8.37720000
H	8.81426000	6.98946600	6.69500000
H	11.21640000	6.95631200	7.39778000
H	17.18574000	6.71053400	19.30500000
H	18.99170000	6.72108300	17.62280000
H	19.30838000	6.85822000	8.81374000
H	15.18088000	6.91822600	7.53740000
H	17.62670000	6.90397800	7.00752000
N	14.30806000	6.81465400	14.40504000
N	12.87936000	6.79739200	16.36414000
N	11.59366000	6.84164300	14.30962000
N	9.63612000	6.88411300	12.88066000

N	11.69194000	6.88562000	11.59496000
N	14.40634000	6.85863100	11.69038000
N	16.36388000	6.81602400	13.11934000
N	13.12064000	6.90288200	9.63586000

NiPc from PBE

C	15.32388000	6.77423900	16.54068000
C	16.35712000	6.77834900	15.58258000
C	15.71258000	6.80506400	14.27478000
C	14.06834000	6.79574800	15.79994000
C	11.72470000	6.81465400	15.71180000
C	10.19928000	6.85438400	14.06834000
C	10.41716000	6.81712000	16.35686000
C	9.45880000	6.84178000	15.32440000
C	10.28742000	6.89521000	11.72522000
C	10.67612000	6.92589800	9.45932000
C	9.64288000	6.92178800	10.41742000
C	14.27530000	6.88562000	10.28820000
C	15.80072000	6.84589000	11.93166000
C	16.54120000	6.85876800	10.67560000
C	15.58284000	6.88329100	9.64314000
C	11.93166000	6.90438900	10.20006000
C	15.60754000	6.75204500	17.90438000
C	17.69586000	6.75807300	15.96764000
C	10.03262000	6.80232400	17.69586000
C	8.09510000	6.85219200	15.60936000
C	17.90490000	6.84849300	10.39064000
C	15.96738000	6.89808700	8.30414000
C	7.71212000	6.83821800	16.94940000

C	8.66814000	6.81355800	17.97900000
C	8.30414000	6.94206400	10.03236000
C	8.02256000	6.96466900	8.66762000
C	9.05268000	6.96699800	7.71212000
C	10.39246000	6.94809200	8.09562000
C	16.94732000	6.73313900	18.28788000
C	17.97744000	6.73533100	17.33238000
C	17.33186000	6.88699000	8.02100000
C	18.28788000	6.86246700	9.05060000
H	14.80414000	6.74944200	18.63810000
H	18.48782000	6.75971700	15.22170000
H	10.77934000	6.78328100	18.48730000
H	7.36060000	6.87109800	14.80674000
H	18.63940000	6.82958700	11.19326000
H	6.65418000	6.84684900	17.20680000
H	8.33352000	6.80342000	19.01510000
H	7.51218000	6.94028300	10.77856000
H	6.98672000	6.98124600	8.33248000
H	8.79632000	6.98439700	6.65392000
H	11.19586000	6.95069500	7.36190000
H	17.20368000	6.71574000	19.34608000
H	19.01328000	6.71875400	17.66778000
H	19.34582000	6.85383600	8.79320000
H	15.22066000	6.91699300	7.51270000
H	17.66648000	6.89712800	6.98490000
N	14.35122000	6.81369500	14.45600000
N	12.87312000	6.79629600	16.37662000
N	11.54348000	6.83630000	14.35044000
N	9.62234000	6.88123600	12.87338000
N	11.64878000	6.88644200	11.54400000

N	14.45652000	6.86397400	11.64956000
N	16.37766000	6.81903800	13.12662000
N	13.12688000	6.90384100	9.62338000
Ni	13.00000000	6.85013700	13.00000000

CuPc from PBE

C	15.32050000	6.77300600	16.52274000
C	16.34984000	6.77862300	15.56438000
C	15.70192000	6.80602300	14.26100000
C	14.06652000	6.79684400	15.78408000
C	11.73848000	6.81986000	15.70166000
C	10.21566000	6.86013800	14.06652000
C	10.43484000	6.82218900	16.34984000
C	9.47674000	6.84767100	15.32076000
C	10.29808000	6.89644300	11.73874000
C	10.67924000	6.92904900	9.47700000
C	9.65016000	6.92329500	10.43536000
C	14.26152000	6.88383900	10.29834000
C	15.78434000	6.84356100	11.93322000
C	16.52326000	6.85630200	10.67898000
C	15.56516000	6.88164700	9.65016000
C	11.93348000	6.90575900	10.21592000
C	15.60494000	6.74848300	17.88644000
C	17.68988000	6.75971700	15.94554000
C	10.05342000	6.80451600	17.68988000
C	8.11278000	6.85630200	15.60520000
C	17.88722000	6.84780800	10.39454000
C	15.94632000	6.89945700	8.31012000
C	7.73188000	6.83835500	16.94498000

C	8.68946000	6.81273600	17.97354000
C	8.30986000	6.94137900	10.05420000
C	8.02620000	6.96508000	8.69050000
C	9.05476000	6.97083400	7.73266000
C	10.39480000	6.95288700	8.11330000
C	16.94472000	6.72985100	18.26708000
C	17.97354000	6.73546800	17.30950000
C	17.31028000	6.89151100	8.02620000
C	18.26812000	6.86589200	9.05476000
Cu	13.00000000	6.85164400	13.00000000
H	14.80232000	6.74423600	18.62120000
H	18.48028000	6.76437500	15.19804000
H	10.80092000	6.78478800	18.48002000
H	7.37828000	6.87630400	14.80284000
H	18.62172000	6.82780600	11.19690000
H	6.67446000	6.84410900	17.20394000
H	8.35562000	6.79903600	19.00990000
H	7.51946000	6.93672100	10.80196000
H	6.98984000	6.97932800	8.35692000
H	8.79606000	6.98960300	6.67550000
H	11.19716000	6.95727100	7.37854000
H	17.20342000	6.71053400	19.32450000
H	19.00990000	6.72039800	17.64334000
H	19.32554000	6.86027500	8.79580000
H	15.19882000	6.91918500	7.51972000
H	17.64438000	6.90534800	6.98984000
N	14.33640000	6.81602400	14.43442000
N	12.88014000	6.79876200	16.37194000
N	11.56532000	6.84246500	14.33614000
N	9.62754000	6.88466100	12.88040000

N	11.66360000	6.88657900	11.56532000
N	14.43468000	6.86123400	11.66360000
N	16.37220000	6.81835300	13.11934000
N	13.11986000	6.90438900	9.62780000

ZnPc from PBE

C	15.33662000	6.77245800	16.54614000
C	16.36934000	6.77807500	15.58466000
C	15.72272000	6.80492700	14.27660000
C	14.07822000	6.79588500	15.80722000
C	11.72288000	6.81794200	15.72246000
C	10.19226000	6.85835700	14.07848000
C	10.41482000	6.81999700	16.36960000
C	9.45308000	6.84561600	15.33688000
C	10.27728000	6.89534700	11.72340000
C	10.66338000	6.92767900	9.45386000
C	9.63066000	6.92206200	10.41534000
C	14.27712000	6.88233200	10.27754000
C	15.80774000	6.84191700	11.92152000
C	16.54692000	6.85465800	10.66312000
C	15.58518000	6.88027700	9.63040000
C	11.92178000	6.90438900	10.19278000
C	15.62496000	6.74766100	17.90906000
C	17.70860000	6.75916900	15.96894000
C	10.03028000	6.80218700	17.70860000
C	8.09016000	6.85424700	15.62548000
C	17.90984000	6.84616400	10.37452000
C	15.96972000	6.89808700	8.29140000
C	7.70874000	6.83616300	16.96578000

C	8.66606000	6.81040700	17.99382000
C	8.29140000	6.94096800	10.03106000
C	8.006444000	6.96535400	8.66736000
C	9.03474000	6.97110800	7.70978000
C	10.37504000	6.95247600	8.09094000
C	16.96526000	6.72889200	18.29022000
C	17.99356000	6.73464600	17.33264000
C	17.33368000	6.89000400	8.00618000
C	18.29126000	6.86424800	9.03422000
H	14.82312000	6.74314000	18.64486000
H	18.49926000	6.76369000	15.22144000
H	10.77752000	6.78232200	18.49926000
H	7.35436000	6.87424900	14.82390000
H	18.64564000	6.82602500	11.17610000
H	6.65106000	6.84191700	17.22448000
H	8.33300000	6.79657000	19.03044000
H	7.50074000	6.93644700	10.77856000
H	6.96982000	6.98042400	8.33430000
H	8.77630000	6.99056200	6.65210000
H	11.17688000	6.95686000	7.35514000
H	17.22370000	6.70943800	19.34790000
H	19.03018000	6.71957600	17.66570000
H	19.34894000	6.85863100	8.77552000
H	15.22248000	6.91808900	7.50074000
H	17.66700000	6.90397800	6.96956000
N	14.36084000	6.81451700	14.46224000
N	12.87832000	6.79780300	16.38104000
N	11.53724000	6.84027300	14.36084000
N	9.61818000	6.88329100	12.87884000
N	11.63916000	6.88575700	11.53802000

N	14.46276000	6.86000100	11.63916000
N	16.38156000	6.81698300	13.12116000
N	13.12168000	6.90233400	9.61896000
Zn	13.00000000	6.85013700	13.00000000

H₂Pc-MoS₂

C	9.78107299	4.00776989	21.31407002
C	11.00089304	4.70496033	21.30971214
C	10.64615368	6.12498610	21.31718279
C	8.73787772	5.03436171	21.32247450
C	6.46095755	5.58899208	21.33181281
C	5.31662101	7.57161247	21.33368047
C	5.04431758	5.27663419	21.35889391
C	4.33732187	6.50137656	21.35858263
C	5.98653711	9.81561956	21.32527599
C	6.85261100	11.93219864	21.31095725
C	5.63212882	11.23532676	21.31189108
C	10.17289197	10.35209144	21.32870004
C	11.31623531	8.36899319	21.32216322
C	12.29636212	9.43891053	21.34301878
C	11.58969748	10.66381218	21.34613155
C	7.89530966	10.90592538	21.32371961
C	9.74548318	2.61625613	21.30846703
C	12.21723687	4.02911407	21.29819489
C	4.36794566	4.05635181	21.38597501
C	2.94203578	6.52351718	21.38317351
C	13.69181374	9.41565492	21.36294051
C	12.26805581	11.88377600	21.36667583
C	2.27394056	5.30419050	21.40465163

C	2.97779113	4.08566025	21.40651929
C	4.41611605	11.91228801	21.29788362
C	4.45170586	13.30778390	21.27951827
C	5.67020164	14.00338149	21.27889572
C	6.88935955	13.32339383	21.29601596
C	10.96513769	1.93722417	21.29321446
C	12.18297133	2.63345890	21.28730020
C	13.65821034	11.85319327	21.38099458
C	14.36123324	10.63434445	21.37974947
H	7.43479408	7.47540434	21.29134680
H	9.19756564	8.46663489	21.29508212
H	8.79796657	2.08089924	21.31064597
H	13.15945640	4.57355021	21.29165808
H	4.91818067	3.11768530	21.38472990
H	2.40289154	7.46855508	21.38037202
H	14.23046138	8.47013916	21.35889391
H	1.18505791	5.28746558	21.40216141
H	2.41977601	3.15065730	21.40714184
H	3.47323439	11.36880759	21.29414829
H	3.51925284	13.86958209	21.25430484
H	5.66076620	15.09193518	21.25399356
H	7.83737276	13.85763572	21.29321446
H	10.97556634	0.84835191	21.27360401
H	13.11575542	2.07245714	21.26333187
H	15.45011589	10.65027295	21.37383520
H	11.71881400	12.82307964	21.36636456
H	14.21721866	12.78771837	21.37383520
Mo	9.19044768	3.17614290	16.44445263
Mo	11.94874072	1.58377075	16.46686458
Mo	9.19028215	6.36200218	16.42670984

Mo	11.94989946	4.76851505	16.44414136
Mo	9.18862681	9.54340149	16.42702112
Mo	11.94989946	7.95198505	16.43635943
Mo	9.18995108	12.73101291	16.44725413
Mo	11.94526451	11.13880005	16.44320753
Mo	9.18978554	15.91910218	16.46406308
Mo	11.94691985	14.32227006	16.46779841
Mo	14.70852357	3.17630218	16.47464650
Mo	0.91623069	1.58345218	16.48273970
Mo	14.70902017	6.36025005	16.46126159
Mo	0.91772050	4.76915219	16.46966607
Mo	14.70620609	9.54308292	16.45877138
Mo	0.91672729	7.95421504	16.46717585
Mo	14.70587503	12.72910149	16.46997735
Mo	0.91424428	11.13800362	16.47122245
Mo	14.70736483	15.91766862	16.47962693
Mo	0.91391321	14.32338505	16.47931566
Mo	3.67684121	3.17709861	16.46468564
Mo	6.43281677	1.58377075	16.46095031
Mo	3.67485480	6.36391360	16.44632029
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S	8.27388592	1.59173501	18.02013681
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S	11.02671634	15.91862433	18.02916384
S	8.27057524	4.76039151	14.87312634
S	8.27487913	4.77743500	17.99087677
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S	11.02257799	3.18904498	18.00270530
S	8.27123738	7.95246291	14.86316547
S	8.27322379	7.95278148	17.99336698
S	11.03697945	6.35626793	14.87188123
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S	11.03515858	9.54754290	14.87250378
S	11.02158479	9.54164935	17.98683017
S	8.27040971	14.33119002	14.89647211
S	8.27206505	14.31717294	18.01951425
S	11.03267557	12.74120715	14.89086913
S	11.02092265	12.71986296	18.01609021
S	13.79378269	1.58058506	14.91390362
S	13.78269191	1.58552289	18.03538938
S	16.54959272	15.91926147	14.92106299
S	16.54859951	15.91719076	18.04192620
S	13.80040405	4.76134722	14.89896233

S	13.77756035	4.77536430	18.02231575
S	16.55058592	3.17056792	14.91670512
S	16.55075146	3.18283287	18.03943598
S	13.79941084	7.95007363	14.89024657
S	13.77623608	7.95166648	18.01484510
S	0.00016553	6.35929434	14.90643298
S	16.54909612	6.36311718	18.03040895
S	13.79527249	11.14118932	14.89491573
S	13.77275987	11.12940224	18.00799700
S	16.55191019	9.54754290	14.90643298
S	16.54379903	9.54419791	18.03040895
S	13.79080307	14.32720789	14.91359235
S	13.78252637	14.31781008	18.03663449
S	16.54959272	12.73419861	14.91421490
S	16.54495777	12.72511936	18.03725704
S	2.74935421	1.57962934	14.91514873
S	2.76226586	1.58966430	18.03881343
S	5.50566084	15.91989861	14.90518787
S	5.52088997	15.91766862	18.02760746
S	2.74968527	4.76182507	14.89740594
S	2.76656974	4.77886857	18.01204360
S	5.50748171	3.16706366	14.89335934
S	5.52287638	3.18585928	18.01858042
S	2.74554692	7.95596718	14.89242551
S	2.76640421	7.95596718	18.01702404
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S	5.52188317	6.36757716	17.98932038
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S	5.50317783	9.54674648	14.87125867

S	5.52436618	9.54658719	17.98932038
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CoPc-MoS₂

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C	6.45433619	5.63215831	18.69685301
C	5.34310645	7.55807325	18.69996577
C	5.04497972	5.29240341	18.74478966
C	4.34377769	6.50695153	18.74541222
C	5.94465701	9.78264756	18.70214471
C	6.82380808	11.89189953	18.72829198
C	5.60796085	11.19279767	18.72984837
C	10.10005701	10.29697883	18.69934322
C	11.21012801	8.37010818	18.69623045
C	12.21011891	9.42027419	18.74105434
C	11.51007562	10.63530017	18.74198817
C	7.87329364	10.89190830	18.70027705
C	9.69499531	2.64301600	18.75101520
C	12.16691453	4.06320106	18.74945882
C	4.37556022	4.06957247	18.78774589
C	2.94998141	6.53721568	18.78650078
C	13.60374965	9.38746148	18.77871886
C	12.18214366	11.85717540	18.77716247

C	2.28006532	5.31629616	18.81513827
C	2.98341928	4.09856233	18.81638337
C	4.38665100	11.86482108	18.74790243
C	4.41942673	13.25792769	18.75039265
C	5.63858464	13.95878169	18.74852499
C	6.85840469	13.28548399	18.74478966
C	10.91498089	1.96939974	18.75786330
C	12.13397327	2.67009446	18.75692947
C	13.57445014	11.82595554	18.79832931
C	14.27598323	10.60710672	18.79988569
Co	8.27686553	7.96440928	18.58354818
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H	13.10615445	4.61289360	18.75537308
H	4.92761611	3.13170239	18.79179249
H	2.41216145	7.48320930	18.78867972
H	14.13958321	8.44019358	18.78276546
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H	2.42556970	3.16292224	18.82167508
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H	3.48531837	13.81765518	18.74510094
H	5.62467979	15.04765395	18.74105434
H	7.80641791	13.82004445	18.74883626
H	10.92855468	0.88052748	18.75506180
H	13.06791610	2.11020768	18.75350542
H	15.36519695	10.62096451	18.79895186
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Mo	11.95536208	4.77855000	13.90505487
Mo	9.19458603	9.55550715	13.90007444
Mo	11.95602422	7.96393143	13.89353762
Mo	9.19392389	12.74295928	13.90194210
Mo	11.95072713	11.15074642	13.89633911
Mo	9.19491710	0.00095571	13.91532701
Mo	11.95221694	14.33453500	13.92061872
Mo	14.71398619	3.18649643	13.93369235
Mo	0.92020351	1.59444285	13.94147428
Mo	14.71481386	6.37140000	13.91314807
Mo	0.92252098	4.78014285	13.92279766
Mo	14.71117211	9.55502930	13.90661125
Mo	0.92086564	7.96520571	13.91501573
Mo	14.71050998	12.74072929	13.92279766
Mo	0.91755496	11.14979071	13.92279766
Mo	14.71233085	15.92834072	13.93773895
Mo	0.91805156	14.33565000	13.93711640
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Mo	6.43778279	1.59412428	13.91470445
Mo	3.67932422	6.37570069	13.90163082
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S	11.03880032	0.00238927	12.35956456
S	11.03002702	15.92706643	15.48385181
S	8.27852087	4.77791286	12.33808645
S	8.27785874	4.78046142	15.45241283
S	11.04161440	3.17901003	12.34649093
S	11.02820615	3.19669067	15.46112859
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S	11.03615178	6.36646216	12.33684134
S	11.03582071	6.37570069	15.45085645
S	8.27967961	11.15090571	12.33279474
S	8.26958204	11.14835715	15.44743240
S	11.03333770	9.55773714	12.33248346
S	11.03631731	9.55582572	15.44556474
S	8.27305825	14.34138426	12.34866987
S	8.27703107	14.33023431	15.47326839
S	11.03631731	12.75251638	12.34368943
S	11.02655081	12.73276505	15.46797668
S	13.79974191	1.59141643	12.37232692
S	13.78716133	1.59555784	15.49536906
S	16.55306893	0.00238927	12.37979757
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S	13.80321812	4.77010789	12.35707435

S	13.78583705	4.78794781	15.48042776
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S	0.00297961	3.19557567	15.49723672
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S	13.78649919	7.96520571	15.46642030
S	0.00446942	6.36757716	12.35582924
S	0.00099320	6.37585998	15.48167287
S	13.79858317	11.15488784	12.34493454
S	13.78020890	11.13975576	15.45801582
S	0.00264854	9.56076356	12.35365030
S	16.54628204	9.55327716	15.47918266
S	13.79808657	14.34074712	12.36796904
S	13.78633366	14.32704861	15.49194501
S	0.00016553	12.74917140	12.36796904
S	16.54777184	12.73499504	15.49194501
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S	2.76805955	1.60065496	15.49630289
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S	5.52668366	15.92786286	15.48385181
S	2.75680324	4.77361217	12.35147136
S	2.77004596	4.79065566	15.46517519
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S	5.52320744	9.56315283	15.45054517
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NiPc-MoS₂

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C	6.46128862	5.63868900	18.77996396
C	5.35187975	7.56125895	18.78214290
C	5.05226321	5.29861552	18.79428271
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C	5.95127837	9.77532045	18.77965269
C	6.82744983	11.88234243	18.77622864
C	5.61375454	11.18371842	18.77965269
C	10.09343565	10.29044814	18.77467225
C	11.20168578	8.36708177	18.77062565
C	12.20184221	9.41597349	18.78152035
C	11.50279213	10.62956590	18.78276546
C	7.87627325	10.88298834	18.77591736
C	9.69151910	2.65241382	18.77871886
C	12.16327279	4.07498815	18.77591736
C	4.38300925	4.07498815	18.80113080
C	2.95809258	6.54406494	18.79957441
C	13.59613509	9.38172721	18.78214290
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C	2.99103385	4.10509302	18.80953528
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C	4.42257188	13.24566275	18.76782416
C	5.64156425	13.94763174	18.76408884
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C	13.56600790	11.82053985	18.78401057
C	14.26787206	10.60137246	18.78463312
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H	13.10102290	4.62659211	18.76440011
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H	10.92640274	0.89167743	18.76066479
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Mo	9.19524817	6.37347070	13.86521141
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Mo	14.71431726	3.18729285	13.91159168
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Mo	14.71448279	6.37155928	13.89727294
Mo	0.92384525	4.78062070	13.90567742
Mo	14.71067551	9.55502930	13.89291506
Mo	0.92169331	7.96520571	13.90194210
Mo	14.70902017	12.74009216	13.90380976
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Mo	14.71199978	15.92802214	13.91688339
Mo	0.91755496	14.33501286	13.91719467
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N	6.62169107	7.01252212	18.77124821
N	5.02792972	8.83665395	18.78650078

N	7.32521057	9.61396475	18.76938055
N	9.93220553	8.91629645	18.76471139
N	11.52596689	7.09152748	18.77685119
N	9.15154719	11.21000045	18.77965269
Ni	8.27703107	7.96440928	18.74292200
S	8.27471359	1.58695645	12.33559623
S	8.27686553	1.60113282	15.46019476
S	11.03548964	0.00254856	12.34493454
S	11.03135129	15.92738500	15.46797668
S	8.27752767	4.77074504	12.31225046
S	8.27852087	4.78985923	15.43124600
S	11.04029013	3.17821361	12.33030452
S	11.02770955	3.19955780	15.44525346
S	8.27703107	7.96249786	12.29824299
S	8.27785874	7.96504642	15.42751067
S	11.04227654	6.36550645	12.31069407
S	11.02671634	6.37681569	15.42937834
S	8.27653447	11.15775496	12.30820386
S	8.27454806	11.13927791	15.42688812
S	11.04012460	9.55837428	12.30664747
S	11.02638527	9.55264002	15.42346407
S	8.27355485	14.34393282	12.33403985
S	8.27686553	14.32704861	15.45863837
S	11.03615178	12.75267567	12.32532409
S	11.02572314	12.73165005	15.44992262
S	13.79792104	1.59077929	12.35271647
S	13.78931327	1.59651356	15.47482478
S	16.55273786	0.00095571	12.35863073
S	16.55240680	15.92818143	15.47949393
S	13.80437686	4.77265645	12.33715262

S	13.78633366	4.78635496	15.46143987
S	0.00231748	3.18187716	12.35271647
S	0.00297961	3.19366425	15.47544733
S	13.80437686	7.96090501	12.32532409
S	13.78202977	7.96329429	15.45023390
S	0.00430388	6.37028501	12.34213305
S	0.00082767	6.37490427	15.46642030
S	13.80023851	11.15297641	12.32750303
S	13.77838802	11.14103004	15.44027303
S	0.00331068	9.55869285	12.34088794
S	16.54727524	9.55455144	15.46548647
S	13.79543803	14.34090640	12.34804731
S	13.78583705	14.32768575	15.47202329
S	0.00033107	12.74678212	12.34991498
S	16.54644757	12.73547289	15.47295712
S	2.75465129	1.58870859	12.35053753
S	2.76756295	1.60129210	15.47451350
S	5.51112346	0.00079643	12.34400071
S	5.52486278	0.00015929	15.46704285
S	2.75547896	4.77456787	12.33279474
S	2.77302557	4.78906281	15.44649857
S	5.51459968	3.17773575	12.32905942
S	5.52684919	3.19700923	15.45459177
S	2.75233382	7.96727642	12.32843686
S	2.77070809	7.96727642	15.45303539
S	5.51377201	6.36805501	12.31100535
S	5.52784240	6.37856782	15.42813323
S	2.75150615	11.15632140	12.33684134
S	2.76574207	11.14341932	15.46112859
S	5.50996472	9.56012641	12.31007152

S	5.52883560	9.55439215	15.42906706
S	2.75266489	14.34090640	12.35116008
S	2.76359013	14.33023431	15.47357967
S	5.50963366	12.75283495	12.32719175
S	5.52668366	12.72830506	15.44182942

CuPc-MoS₂

C	9.74300017	4.00999987	18.78836844
C	10.96149595	4.71260601	18.78587823
C	10.62297892	6.12785323	18.78276546
C	8.68755539	5.01126538	18.78587823
C	6.43827940	5.61527411	18.78618950
C	5.32357344	7.55074614	18.78899100
C	5.02312923	5.27743062	18.80081952
C	4.32076847	6.49627944	18.80113080
C	5.93009002	9.80096534	18.78743461
C	6.81023429	11.91865941	18.78214290
C	5.59157299	11.21557542	18.78494440
C	10.11512060	10.31418160	18.77747375
C	11.22932996	8.37823171	18.77529481
C	12.23246600	9.43253913	18.78432184
C	11.53043630	10.65154724	18.78463312
C	7.86551354	10.91755318	18.78214290
C	9.71353512	2.61657469	18.78774589
C	12.18181259	4.03962688	18.78120907
C	4.35039905	4.05682967	18.80548868
C	2.92713772	6.52463217	18.80424357
C	13.62626228	9.40323069	18.78276546
C	12.20432522	11.87182962	18.78120907

C	2.25540075	5.30403122	18.81295933
C	2.95759598	4.08645667	18.81389316
C	4.37092527	11.88855454	18.78152035
C	4.40105246	13.28166115	18.77809630
C	5.61855503	13.98394872	18.77529481
C	6.83936828	13.31208459	18.77560609
C	10.93434837	1.94439199	18.78650078
C	12.15168541	2.64636099	18.78245418
C	13.59712829	11.84140619	18.78338801
C	14.29866139	10.62335379	18.78432184
Cu	8.27636893	7.96456857	18.73171603
H	8.76684617	2.08010282	18.78338801
H	13.12072144	4.58963799	18.77093693
H	4.90063407	3.11816316	18.79397143
H	2.38981436	7.47094436	18.79148121
H	14.16292351	8.45675922	18.76938055
H	1.16635256	5.28937699	18.79926314
H	2.39891873	3.15145373	18.80113080
H	3.43218196	11.33854344	18.77747375
H	3.46611643	13.84011436	18.77093693
H	5.60349143	15.07298026	18.76626778
H	7.78589169	13.84871576	18.76657905
H	10.94924643	0.85536045	18.78089780
H	13.08662144	2.08790778	18.77311587
H	15.38754404	10.63753016	18.76471139
H	11.65442127	12.81049613	18.76657905
H	14.15580554	12.77609056	18.76128734
Mo	9.19541370	3.18729285	13.88139782
Mo	11.95238247	1.59571713	13.89416017
Mo	9.19557923	6.37187786	13.87859632

Mo	11.95337567	4.77950571	13.88108654
Mo	9.19442050	9.55518858	13.87735121
Mo	11.95387228	7.96377215	13.87797377
Mo	9.19359283	12.74168501	13.88482186
Mo	11.95006499	11.14931286	13.87548355
Mo	9.19425496	0.00079643	13.89540528
Mo	11.95138927	14.33421644	13.89322634
Mo	14.71348959	3.18729285	13.89696167
Mo	0.92152778	1.59444285	13.89820677
Mo	14.71431726	6.37140000	13.89073613
Mo	0.92500399	4.78077999	13.89104740
Mo	14.71034444	9.55455144	13.88544442
Mo	0.92252098	7.96504642	13.89571656
Mo	14.71017891	12.73865859	13.88855719
Mo	0.91970690	11.14867572	13.89602783
Mo	14.71233085	15.92818143	13.89633911
Mo	0.91987244	14.33437572	13.89665039
Mo	3.68296597	3.18904498	13.88700080
Mo	6.43794833	1.59380571	13.89073613
Mo	3.68147616	6.37554141	13.87859632
Mo	6.43827940	4.77982428	13.88015271
Mo	3.68081402	9.55741857	13.88575569
Mo	6.43943813	7.96440928	13.87859632
Mo	3.68081402	12.74136643	13.89011357
Mo	6.43778279	11.14835715	13.86956929
Mo	3.67998635	15.92834072	13.89789550
Mo	6.43712066	14.33342001	13.89042485
N	9.25417827	6.26515691	18.77280459
N	7.39936980	4.70416390	18.79272632
N	6.57732796	6.98401011	18.77404970

N	5.01932195	8.83936179	18.79615037
N	7.29889066	9.66382095	18.77498353
N	9.97557544	8.94528632	18.76533395
N	11.53374698	7.08929750	18.78432184
N	9.15386467	11.22481395	18.78525567
S	8.27487913	1.58711574	12.32843686
S	8.27736214	1.60065496	15.45210156
S	11.03300663	0.00031857	12.33528496
S	11.03433091	0.00111499	15.45739327
S	8.27636893	4.77870928	12.31691961
S	8.27703107	4.78157641	15.43591515
S	11.03648285	3.18251430	12.32127749
S	11.02953042	3.19509781	15.43840537
S	8.27653447	7.96297572	12.31629706
S	8.27752767	7.96345357	15.44245197
S	11.03482751	6.37108143	12.31629706
S	11.03317217	6.37331142	15.43498132
S	8.28166602	11.15138356	12.31411812
S	8.27024417	11.14485288	15.43280238
S	11.03251003	9.55439215	12.31380684
S	11.03300663	9.55678143	15.43093472
S	8.27636893	14.34042855	12.32968197
S	8.27521019	14.33055288	15.45365794
S	11.03118576	12.75124210	12.32190004
S	11.02969595	12.73419861	15.44587602
S	13.79510696	1.59380571	12.33559623
S	13.79063754	1.59396500	15.45708199
S	0.00066214	0.00079643	12.33777517
S	0.00016553	15.92818143	15.45708199
S	13.80123172	4.77695715	12.32905942

S	13.78699579	4.78237284	15.45147900
S	0.00049660	3.18474429	12.33528496
S	0.00413835	3.19159354	15.45739327
S	13.79874871	7.95883431	12.32252260
S	13.78782346	7.96409071	15.44649857
S	0.00314515	6.37442641	12.33341729
S	0.00314515	6.37044429	15.45645943
S	13.79543803	11.14803858	12.31972111
S	13.78236084	11.14389717	15.43342494
S	0.00430388	9.55598500	12.33341729
S	16.54727524	9.55550715	15.45645943
S	13.79163074	14.33772070	12.33279474
S	13.79196181	14.32911931	15.45490305
S	0.00297961	12.74104786	12.33372857
S	16.54793738	12.73977359	15.45583688
S	2.75961731	1.58982358	12.33435112
S	2.76541100	1.60017711	15.45677071
S	5.51559288	0.00063714	12.33341729
S	5.52271084	15.92674786	15.45614816
S	2.76011392	4.77839071	12.32190004
S	2.77037702	4.78699211	15.43716026
S	5.52055890	3.18139930	12.32345643
S	5.52221424	3.19207140	15.44836623
S	2.75415469	7.97062140	12.32407898
S	2.76938382	7.96520571	15.44898879
S	5.52088997	6.37251499	12.31598578
S	5.52006230	6.37394856	15.43373621
S	2.75531343	11.15090571	12.33030452
S	2.76491440	11.14756072	15.45303539
S	5.51393754	9.55248073	12.31474067

S	5.52602152	9.56012641	15.43373621
S	2.75862411	14.33835785	12.33435112
S	2.76226586	14.33055288	15.45645943
S	5.51459968	12.74917140	12.31878728
S	5.52469725	12.73117220	15.43591515

ZnPc-MoS₂

C	9.75094580	3.99024854	18.75568436
C	10.97473867	4.69285467	18.75443925
C	10.63986338	6.11224330	18.73047092
C	8.69401121	4.99406260	18.73202731
C	6.41824978	5.60173488	18.73389497
C	5.29758460	7.54405617	18.73856412
C	4.99995447	5.26261712	18.77187076
C	4.29444856	6.48465164	18.77280459
C	5.91486089	9.81689384	18.74074306
C	6.80344740	11.93888861	18.75692947
C	5.57998561	11.23580461	18.75848585
C	10.13680556	10.32867654	18.73358369
C	11.25631200	8.38539954	18.72891454
C	12.26027571	9.44368908	18.76222118
C	11.55576301	10.66636074	18.76315501
C	7.86071306	10.93555239	18.73856412
C	9.72098415	2.59761978	18.76502267
C	12.19141357	4.01445985	18.76159862
C	4.32573449	4.04297187	18.79895186
C	2.90098335	6.50806653	18.79832931
C	13.65374092	9.41756634	18.78432184
C	12.23263153	11.88489099	18.78245418

C	2.22974298	5.28698772	18.81295933
C	2.93260034	4.07052817	18.81420443
C	4.36248304	11.91356229	18.76097607
C	4.39476217	13.30698747	18.75070393
C	5.61292687	14.00672647	18.74945882
C	6.83225032	13.33199521	18.75817457
C	10.93997653	1.92193281	18.76004224
C	12.15830677	2.62071611	18.75817457
C	13.62576568	11.85494541	18.79085866
C	14.32696770	10.63753016	18.79272632
H	8.77297093	2.06290003	18.76751288
H	13.13230882	4.56144455	18.75973096
H	4.87630057	3.10430537	18.79957441
H	2.36134251	7.45326372	18.79708420
H	14.19139535	8.47141344	18.78556695
H	1.14052926	5.27153708	18.80486612
H	2.37541290	3.13456951	18.80829017
H	3.42224992	11.36578118	18.76190990
H	3.46081934	13.86671496	18.73264986
H	5.60018075	15.09559874	18.73015964
H	7.77976693	13.86751139	18.75630691
H	10.95206051	0.83290127	18.74665732
H	13.09175299	2.06035148	18.74292200
H	15.41618142	10.65122866	18.78214290
H	11.68388632	12.82483177	18.78120907
H	14.18460846	12.78994836	18.77716247
Mo	9.19624137	3.18585928	13.89073613
Mo	11.95354121	1.59364642	13.91532701
Mo	9.19706904	6.37012572	13.87766249
Mo	11.95486548	4.77839071	13.89353762

Mo	9.19557923	9.55694071	13.87579483
Mo	11.95536208	7.96393143	13.87953015
Mo	9.19392389	12.74280000	13.89011357
Mo	11.95138927	11.15042786	13.88388803
Mo	9.19475156	0.00063714	13.90661125
Mo	11.95238247	14.33437572	13.91190296
Mo	14.71348959	3.18649643	13.92559915
Mo	0.92003797	1.59428357	13.93400363
Mo	14.71448279	6.37124071	13.90474359
Mo	0.92235545	4.78014285	13.91501573
Mo	14.71100658	9.55518858	13.89789550
Mo	0.92020351	7.96488714	13.90692253
Mo	14.71067551	12.73993287	13.91532701
Mo	0.91772050	11.14931286	13.91532701
Mo	14.71233085	15.92802214	13.92995703
Mo	0.91821710	14.33533143	13.92933447
Mo	3.68131063	3.18840784	13.91065785
Mo	6.43778279	1.59396500	13.90474359
Mo	3.67849655	6.37490427	13.88855719
Mo	6.43745173	4.77902785	13.88544442
Mo	3.67799995	9.55773714	13.89447145
Mo	6.43678959	7.96440928	13.87890760
Mo	3.67833101	12.74216286	13.91065785
Mo	6.43662406	11.14931286	13.87454972
Mo	3.67866208	0.00031857	13.92435404
Mo	6.43662406	14.33501286	13.90380976
N	9.27255254	6.23903416	18.70494621
N	7.39655572	4.70097821	18.73794157
N	6.54355902	6.96808161	18.70681387
N	5.00889331	8.84222892	18.74541222

N	7.28217173	9.69026226	18.71739729
N	10.01066865	8.96201124	18.70401238
N	11.54516883	7.08674894	18.73420624
N	9.15849962	11.22895536	18.74136562
S	8.27504466	1.58727503	12.33902028
S	8.27885194	1.60065496	15.46424136
S	11.03896586	0.00191142	12.35084881
S	11.02969595	15.92674786	15.47513606
S	8.27703107	4.77217860	12.32065494
S	8.27868641	4.78492140	15.43747154
S	11.04227654	3.17709861	12.33621879
S	11.02671634	3.19764638	15.45147900
S	8.27587233	7.96233858	12.31691961
S	8.27835534	7.96345357	15.44276325
S	11.04128333	6.36471003	12.31972111
S	11.03035809	6.37665641	15.43622643
S	8.27818981	11.15632140	12.31598578
S	8.27156845	11.14341932	15.43280238
S	11.03896586	9.55901142	12.31505195
S	11.03168236	9.55518858	15.42968961
S	8.27289272	14.34281782	12.33839773
S	8.27719660	14.32848217	15.46361881
S	11.03747605	12.75410923	12.33310602
S	11.02621974	12.73037577	15.45739327
S	13.80007298	1.59077929	12.36423372
S	13.78649919	1.59555784	15.48696458
S	16.55306893	0.00222999	12.37232692
S	16.55240680	15.92754429	15.49412395
S	13.80454240	4.76931147	12.34773604
S	13.78351958	4.78842567	15.47140073

S	0.00066214	3.17901003	12.36579010
S	0.00248301	3.19589424	15.48976607
S	13.80437686	7.96026788	12.33123835
S	13.78318851	7.96552428	15.45614816
S	0.00430388	6.36725859	12.34804731
S	0.00033107	6.37570069	15.47389095
S	13.80139725	11.15536569	12.33497368
S	13.77805696	11.13848148	15.44898879
S	0.00264854	9.56076356	12.34586837
S	16.54578544	9.55279930	15.47140073
S	13.79874871	14.34026926	12.36018712
S	13.78616812	14.32641147	15.48416309
S	0.00049660	12.74869355	12.36080967
S	16.54810291	12.73451718	15.48447437
S	2.75216828	1.58918644	12.36454499
S	2.76888722	1.60129210	15.48789841
S	5.50814385	0.00079643	12.35053753
S	5.52784240	15.92786286	15.47451350
S	2.75382362	4.77186003	12.34119922
S	2.77170130	4.79192994	15.45583688
S	5.51178560	3.17853217	12.33839773
S	5.52784240	3.19573495	15.46330753
S	2.75150615	7.96775427	12.33372857
S	2.76805955	7.96536499	15.45894965
S	5.51344094	6.36869215	12.32003238
S	5.52072443	6.37538212	15.43498132
S	2.75150615	11.15775496	12.34617965
S	2.76507994	11.14278218	15.47015562
S	5.50880599	9.55694071	12.31878728
S	5.52618706	9.55853356	15.43560388

S	2.75233382	14.34154355	12.36174350
S	2.76524547	14.32896003	15.48416309
S	5.50781278	12.75363138	12.33217219
S	5.52867007	12.72894220	15.44712113
Zn	8.27703107	7.96520571	18.54526111