ESI for

Determining the Most Promising Anchors for CuSCN: Ab Initio Insights towards p-Type DSSCs

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Surface energies

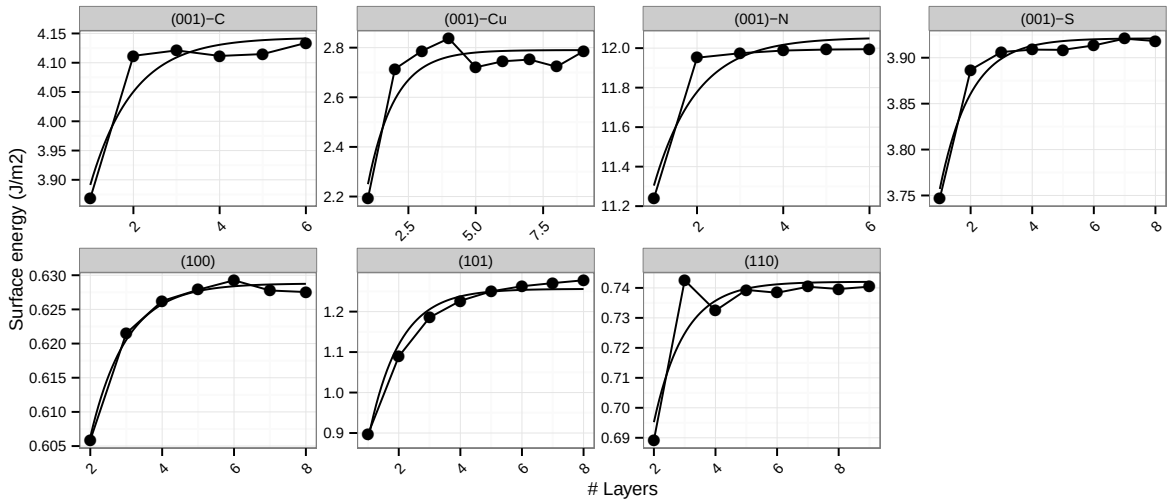

Figure S-1: Convergence of surface energies (J/m^2) with the number of layers.

Comparison of contour plots

The adsorption energies for each combination of anchor and surface are standarized as $(x - \mu)/\sigma$ for a fair scale of comparison. The tables below show the pairwise distances computed for the matrix where the rows correspond to the four monodentate anchors and the columns to each x-y observation on the screening grid. The distance between each anchor is computed as the Euclidean distance, $d = \sqrt{\sum(x_i + y_i)^2}$.

Table S-I: Pairwise distances for anchors on (110)

	aniline	pyridine	thiophenol	thiophenoxide
aniline	–	5.29	4.90	8.78
pyridine	5.29	–	5.89	8.02
thiophenol	4.90	5.89	–	8.39
thiophenoxide	8.78	8.02	8.39	–

Table S-II: Pairwise distances for anchors on (100)

	aniline	pyridine	thiophenol	thiophenoxide
aniline	–	4.44	5.79	7.29
pyridine	4.44	–	5.14	7.03
thiophenol	5.79	5.14	–	7.23
thiophenoxide	7.29	7.03	7.23	–

Binding distances of monodentate anchors

Table S-III: Pairwise distances for anchors on (101)-S

	aniline	pyridine	thiophenol	thiophenoxide
aniline	–	7.88	8.26	7.82
pyridine	7.88	–	6.77	6.85
thiophenol	8.26	6.77	–	7.06
thiophenoxide	7.82	6.85	7.06	–

Table S-IV: Pairwise distances for anchors on (101)-Cu

	aniline	pyridine	thiophenol	thiophenoxide
aniline	–	5.23	4.90	4.67
pyridine	5.23	–	5.04	3.43
thiophenol	4.90	5.04	–	4.18
thiophenoxide	4.67	3.43	4.18	–

Table S-V: Pairwise distances for anchors on (100)

	aniline	pyridine	thiophenol	thiophenoxide
aniline	–	5.75	6.68	7.46
pyridine	5.75	–	6.25	6.33
thiophenol	6.68	6.25	–	5.63
thiophenoxide	7.46	6.33	5.63	–

Table S-VI: Binding distances of monodentate anchor on thick slabs of CuSCN as measured between the anchor heteroatom and the nearest atom of the surface.

Cut	Anchor	Surface atom	Distance (Å)	Binding Energy
(110)	Thiophenoxide	Cu	2.21	0.17
(110)	Thiophenol	Cu	2.48	-0.21
(110)	Pyridine	Cu	2.10	-0.35
(110)	Aniline	N	3.06	-0.01
(100)	Thiophenoxide	Cu	2.19	-0.13
(100)	Thiophenol	Cu	2.31	-0.44
(100)	Pyridine	Cu	2.04	-0.74
(100)	Aniline	Cu	2.18	-0.10
(101)-S	Thiophenoxide	S	2.99	1.00
(101)-S	Thiophenol	S	3.25	0.10
(101)-S	Pyridine	Cu	2.40	0.21
(101)-S	Aniline	C	2.89	0.02
(101)-Cu	Thiophenoxide	Cu	2.19	-3.87
(101)-Cu	Thiophenol	Cu	2.25	-0.92
(101)-Cu	Pyridine	Cu	1.98	-1.55
(101)-Cu	Aniline	Cu	2.04	-1.51
(001)	Thiophenoxide	Cu	2.26	-4.53
(001)	Thiophenol	Cu	2.30	-0.43
(001)	Pyridine	Cu	1.96	-1.12
(001)	Aniline	Cu	2.42	-0.42