DATA for:

Properties of Interfaces Between Copper and Copper Sulphide/Oxide Films

by Joakim Halldin Stenlid, Egon Campos dos Santos, Adam Johannes Johansson, and Lars GM Pettersson

- DFT energies

Structure	**DFT energy / eV**	**Area / Å**
Reference compounds		
Cu_{bulk}	-118.64	N/A
Cu_2O_{bulk}	-217.70	N/A
Cu_2O_{bulk}	-188.60	N/A
CuS_{bulk}	-396.11	N/A
O_2, gas	-9.46	N/A
$S_8, bulk$	-553.35	N/A
Interfaces		
$Cu(100)/Cu_2O(100) : stoi$	-355.47988670	65.3269267820
$Cu(100)/Cu_2O(100) : Cu$	-384.25790522	60.4695804751
$Cu(100)/Cu_2O(100) : O$	-381.41878212	65.7460094607
$Cu(110)/Cu_2O(100) : stoi$	-411.28891326	74.7270120191
$Cu(110)/Cu_2O(100) : Cu$	-447.03575395	74.9339202063
$Cu(110)/Cu_2O(100) : O$	-440.68567105	77.5907675031
$Cu(100)/Cu_2O(110) : stoi$	-269.59996145	40.8549540304
$Cu(100)/Cu_2O(110) : Cu$	-230.26373912	39.0453501185
$Cu(100)/Cu_2O(110) : O$	-254.21205674	41.0305462250
$Cu(110)/Cu_2O(110) : stoi$	-266.32784804	53.0769557761
$Cu(110)/Cu_2O(110) : Cu$	-227.66460967	52.7015119637
$Cu(110)/Cu_2O(110) : O$	-252.59837894	53.5339073474
$Cu(111)/Cu_2O(111) : stoi$	-206.19126116	24.7678963967
$Cu(111)/Cu_2O(111) : Cu$	-195.04899008	23.9818655230
$Cu(111)/Cu_2O(111) : O$	-219.92595292	24.4767487063
$Cu(100)/Cu_2S(100) : stoi$	-336.06807348	50.1489329589
$Cu(100)/Cu_2S(100) : CuS$	-304.80353006	49.9640557084
$Cu(100)/Cu_2S(100) : Cu$	-301.69896094	47.9871414552
$Cu(110)/Cu_2S(100) : stoi$	-500.30506646	95.8017852467
$Cu(110)/Cu_2S(100) : CuS$	-532.79094993	93.9020476646
$Cu(110)/Cu_2S(100) : Cu$	-528.47987177	105.7555442630
$Cu(100)/Cu_2S(110) : stoi$	-263.75269506	48.3695979541
$Cu(111)/Cu_2S(001) : stoi$	-549.77108210	93.0023987892
$Cu(111)/Cu_2S(001) : CuS$	-518.28589411	116.4102286000
$Cu(111)/Cu_2S(001) : Cu$	-583.22771706	127.3539330710
$Cu(111)/CuS : stoi1$	-674.72335339	105.1549008446
$Cu(111)/CuS : Cu$	-586.47216431	98.0904291009
$Cu(111)/CuS : stoi2$	-521.09813302	103.0625980128
$Cu_2O(110) : stoi/Cu_2S(100) : stoi$	-905.25360923	142.3150467880
$Cu_2O(110) : stoi/Cu_2S(100) : CuS$	-958.57645411	143.2853100930
$Cu_2O(110) : stoi/Cu_2S(100) : Cu$	-950.24650147	144.7199981520
$Cu_2O(110) : Cu/Cu_2S(100) : stoi$	-785.12355705	135.7452748990
$Cu_2O(110) : Cu/Cu_2S(100) : CuS$	-840.56268323	144.9074513770
$Cu_2O(110) : Cu/Cu_2S(100) : Cu$	-828.66390961	138.3542440570

Structure	**DFT energy / eV**	**Area / Å**
Interfaces continued		
$Cu_2O(110) : O/Cu_2S(100) : stoi$	-863.54405501	145.9183365690
$Cu_2O(110) : O/Cu_2S(100) : CuS$	-912.31204033	147.5293677920
$Cu_2O(110) : O/Cu_2S(100) : Cu$	-910.19979067	146.7713091190
$Cu_2O(100) : stoi/Cu_2S(100) : stoi$	-604.53467706	99.9776943402
$Cu_2O(100) : stoi/Cu_2S(100) : CuS$	-637.32249772	95.7152571291
$Cu_2O(100) : stoi/Cu_2S(100) : Cu$	-633.68948640	98.8844241477
$Cu_2O(100) : Cu/Cu_2S(100) : stoi$	-647.28684825	98.4087680812
$Cu_2O(100) : Cu/Cu_2S(100) : CuS$	-680.86997848	101.0000644560
$Cu_2O(100) : Cu/Cu_2S(100) : Cu$	-676.12052352	94.9202069190
$Cu_2O(100) : O/Cu_2S(100) : stoi$	-641.96740941	100.9254992470
$Cu_2O(100) : O/Cu_2S(100) : CuS$	-673.55571924	98.7348167047
$Cu_2O(100) : O/Cu_2S(100) : Cu$	-670.84071035	99.6780118452
$Cu_2O(100) : stoi/Cu_2S(110) : stoi$	-952.17041149	163.6933221560
$Cu_2O(100) : Cu/Cu_2S(110) : stoi$	-1018.87945726	162.2458123030
$Cu_2O(100) : O/Cu_2S(110) : stoi$	-1010.43970802	167.4702328930
$Cu_2O(111) : stoi/Cu_2S(001) : stoi$	-859.29443551	116.4723411410
$Cu_2O(111) : stoi/Cu_2S(001) : CuS$	-826.94560269	114.8599584990
$Cu_2O(111) : stoi/Cu_2S(001) : Cu$	-887.50385392	113.1822594870
$Cu_2O(111) : Cu/Cu_2S(001) : stoi$	-805.75033927	103.6236613950
$Cu_2O(111) : Cu/Cu_2S(001) : CuS$	-774.83148100	112.6538284670
$Cu_2O(111) : Cu/Cu_2S(001) : Cu$	-836.66338497	111.4206345500
$Cu_2O(111) : O/Cu_2S(001) : stoi$	-906.44023162	112.9786472850
$Cu_2O(111) : O/Cu_2S(001) : CuS$	-871.06681231	113.9251228890
$Cu_2O(111) : O/Cu_2S(001) : Cu$	-941.72789352	108.2902734180
$Cu_2O(111) : stoi/CuS : stoi1$	-975.99692179	110.1727018777
$Cu_2O(111) : stoi/CuS : Cu$	-898.75305909	108.1877228606
$Cu_2O(111) : stoi/CuS : stoi2$	-831.14233380	111.1034734956
$Cu_2O(111) : Cu/CuS : stoi1$	-933.41485155	109.1116760144
$Cu_2O(111) : Cu/CuS : Cu$	-845.33826945	107.5380902134
$Cu_2O(111) : Cu/CuS : stoi2$	-782.65539599	110.8350660726
$Cu_2O(111) : O/CuS : stoi1$	-1025.33229095	108.7435349727
$Cu_2O(111) : O/CuS : Cu$	-947.19311637	107.5498433436
$Cu_2O(111) : O/CuS : stoi2$	-877.84794899	109.2321000441
Surfaces		
$Cu(100)$	-41.685	12.7
$Cu(110)$	-55.752	18.0
$Cu(111)$	-85.289	22.0
$Cu_2O(100) : O$	-112.978	17.9
$Cu_2O(110) : stoi$	-132.858	25.3
$Cu_2O(110) : Cu$	-110.681	25.3
$Cu_2O(110) : O$	-127.793	25.3

Structure	**DFT energy / eV**	**Area / Å**
Surfaces continued		
$Cu_2O(111) : stoi$	-160.704	31.0
$Cu_2O(111) : Cu$	-169.854	31.0
$Cu_2O(111) : O$	-145.462	31.0
$Cu_2S(100) : stoi$	-114.101	25.0
$Cu_2S(100) : CuS$	-125.654	25.0
$Cu_2S(001) : stoi$	-69.932	13.1
$Cu_2S(001) : Cu$	-71.669	13.1
$Cu_2S(001) : CuS$	-78.876	13.1