Supporting Information to

First principles study of Cu-based inorganic hole transport materials for application in solar cells

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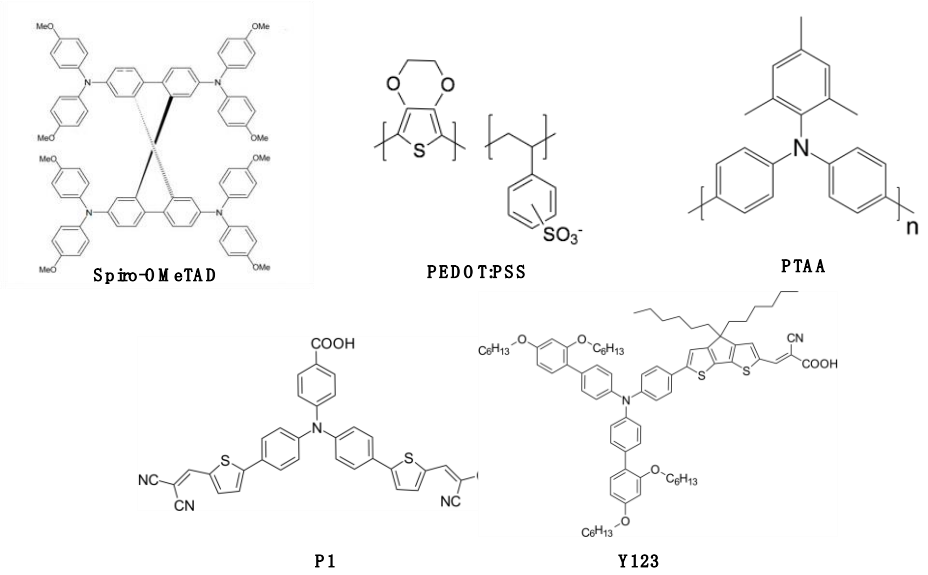

Figure S1: Schematic chemical structures of Spiro-OMeTAD, PEDOT:PSS, PTAA and P1 and Y123 dyes mentioned in this work.

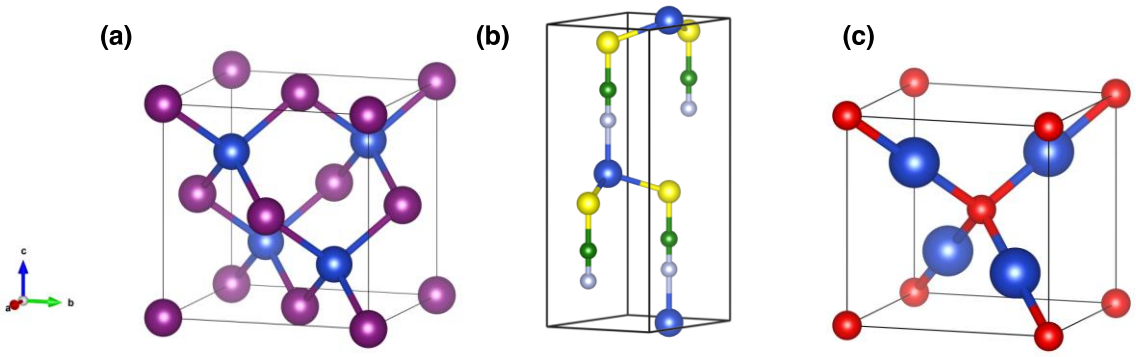

Figure S2: Bulk models shown before relaxation of (a) unit cell of cubic CuI, (b) unit cell hexagonal CuSCN and (c) unit cell of cubic Cu_2O. Color label for atomic spheres: Cu - dark blue; I – violet; S – yellow; C – brown; N – light blue; O – red.

Table S1: Lattice constants of CuI, CuSCN and Cu_2O calculated within the PBE+U level of theory. Experimental values are reported for comparison in the last column.

	Lattice constant (Å)	This work	Exp
CuI	*a*	6.003	6.058[1]
CuSCN	*a*	3.831	3.850
	c	10.883	10.938[2]
Cu_2O	*a*	4.234	4.270[3]

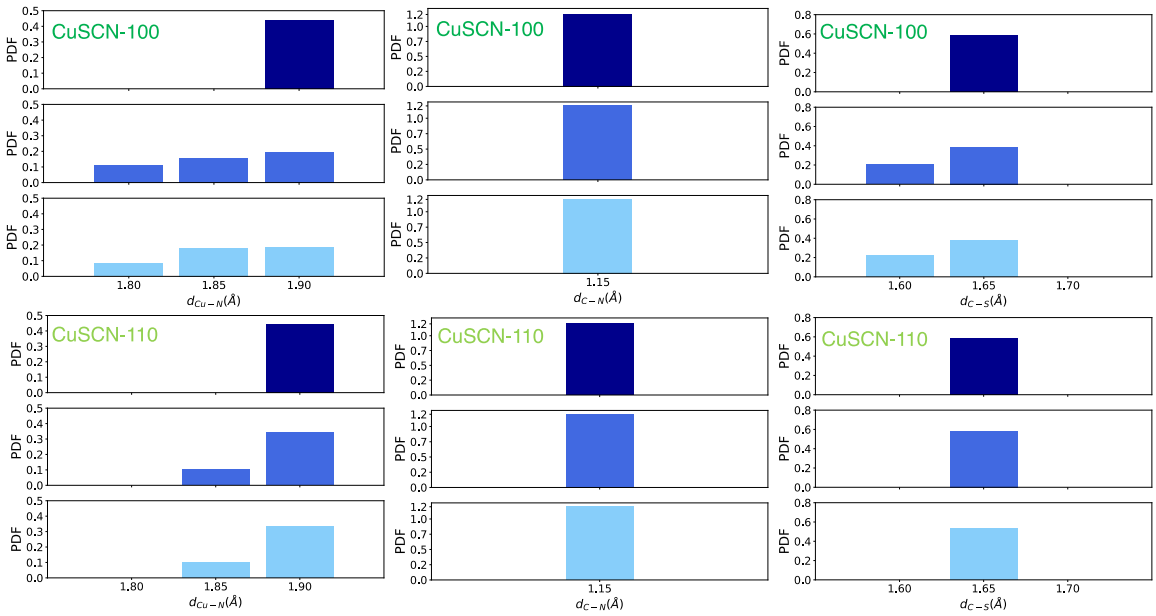

Figure S3: Pair distribution functions of, from left to right: Cu-N, C-N and C-S distances for the CuSCN-100 surface slabs (upper panel) and CuSCN-110 surface slabs (lower panel). Dark blue color is used for structures before relaxation while medium and light blue refer to the pristine and the defective optimized structures, respectively.

References

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[3] A. Sanson, F. Rocca, G. Dalba, P. Fornasini, R. Grisenti, M. Dapiaggi, and G. Artioli, Phys. Rev. B **73**, 214305 (2006).