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Research article

Molecular engineering of fluorinated benzodithiazole-based hole transport materials for efficient perovskite solar cells: A DFT study

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Supplementary

Table S1. A comparison of the energy levels of HOMO, LUMO, and E_g for our designed HTMs with experimentally reported values of well-known HTMs, and perovskite materials.

Molecules	HOMO (eV)	LUMO (eV)	E_g (eV)	Reference
BBT-F2	–4.89	–2.27	2.63	This study
BBT-F4	–4.89	–2.25	2.63	This study
BBT-F6	–5.05	–2.45	2.60	This study
P3HT	–5.00	–3.00	2.00	[1]
PEDOT: PSS	–5.20	–2.00	3.20	[2]
PTAA	–5.10	–1.80	3.30	[3]
SAF-OMe	–5.30	–2.30	3.00	[1]
Spiro-OMeTAD	–5.20	–2.30	2.90	[4]
TTF-1	–5.10	–2.00	3.10	[5]
NiOx	–5.30	–1.80	3.50	[6]
Cu_2O	–5.40	–4.10	1.30	[7]
CuSCN	–5.30	–1.50	3.80	[7]
	CBM	VBM	E_g	
$MAPbI_3$	–3.70	–5.40	1.70	[8]
$FAPbI_3$	–4.00	–5.40	1.40	[9]
$MAPbBr_3$	–3.60	–5.90	2.30	[10]
$MASnI_3$	–4.17	–5.47	1.30	[11]

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