Development of Dopant-Free N, N′-bicarbazole-based Hole Transport Material for Efficient Perovskite Solar Cells

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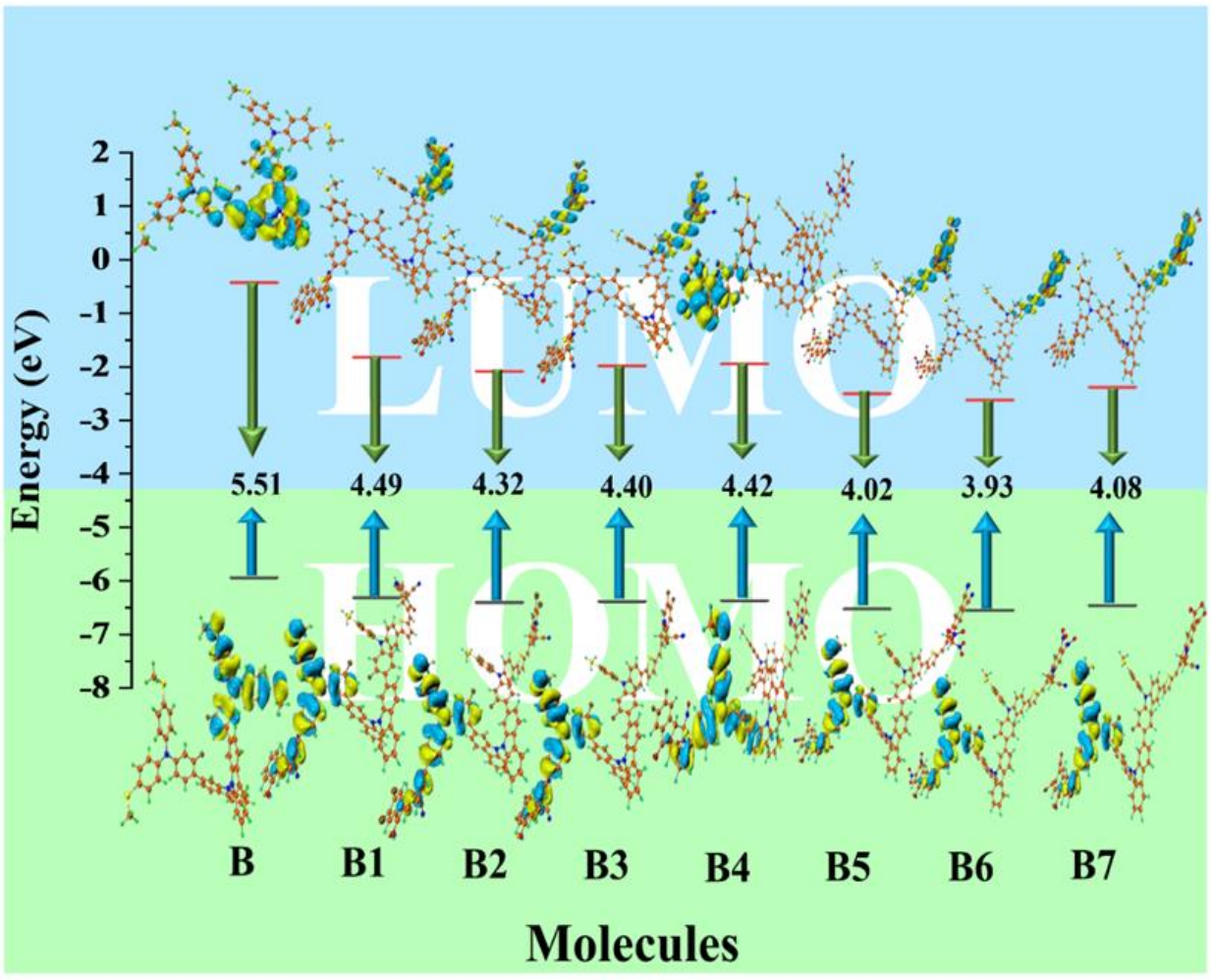


Figure S1: Dispersion of HOMO-LUMO charge density and computed energy gap of synthetic reference B and newly designed B1-B7 HTM series.

Table S1. Computed values of HOMO-LUMO and E_g of newly designed HTM series B1-B7 along with synthetic reference B.

Molecules	(E_{HOMO}) (eV)	(E_{LUMO}) (eV)	$E_g = E_{LUMO} - E_{HOMO}$ (eV)
B	-5.94	-0.43	5.51
B1	-6.31	-1.82	4.49
B2	-6.40	-2.08	4.32
B3	-6.38	-1.99	4.40
B4	-6.37	-1.95	4.42
B5	-6.53	-2.50	4.02
B6	-6.55	-2.62	3.93
B7	-6.46	-2.38	4.08