

Electronic Supporting Information

Effect of substituting donors on Hole Mobility of Hole Transporting Materials in Perovskite Solar Cells

Md Al Mamunur Rashid^a, Sein Min^b, Sung Keon Namgoong^b, Keunhong Jeong^{c,*}

^aClean Energy Research Center, Korea Institute of Science and Technology, Seoul 02792, South Korea

^bDepartment of Chemistry, Seoul Women's University, Seoul 01797, South Korea

^cDepartment of Physics and Chemistry, Korea Military Academy, Seoul, 01805, South Korea

**Corresponding Author: email: doas1mind@berkeley.edu; doas1mind@kma.ac.kr*

Figure S1: Optimized Structures, and HOMO-LUMO of the designed HTMs.

Figure S2: Chemical hardness and Solvation Free energy of the designed HTMs.

Figure S3: Hole and Electron Reorganization Energy of the designed HTMs.

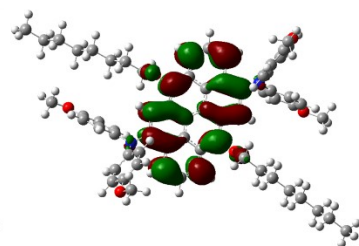
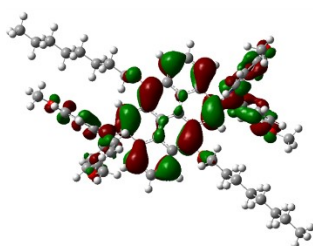
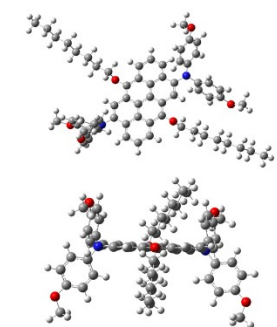
Table S1: Charge transfer Integral, centroid distance, Hole hopping rate, and hole mobility of the designed HTMs.

Optimized Structure

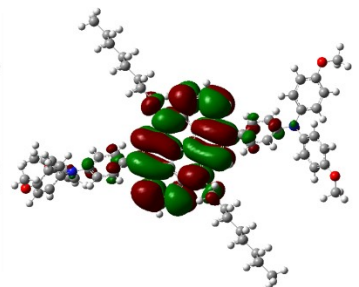
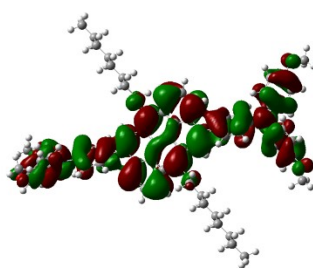
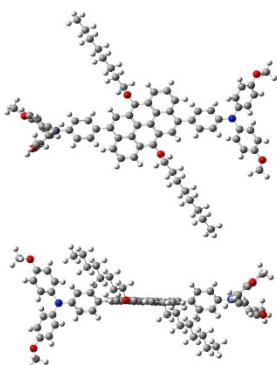
HOMO

LUMO

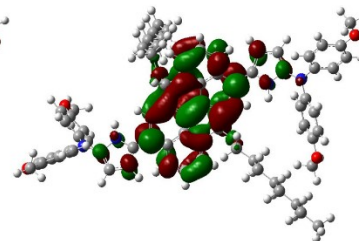
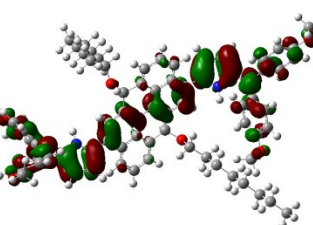
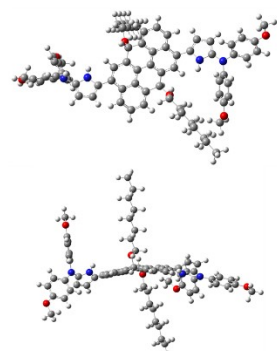
D1



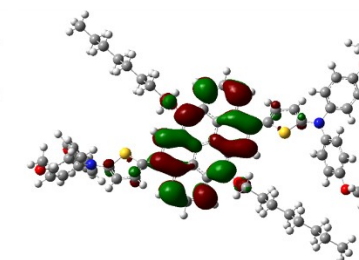
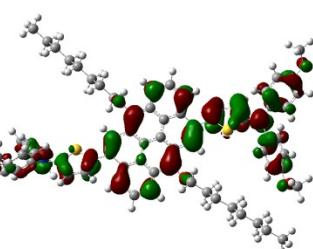
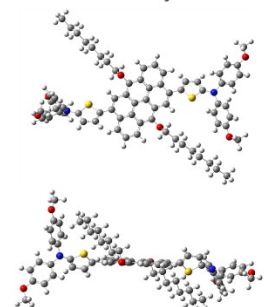
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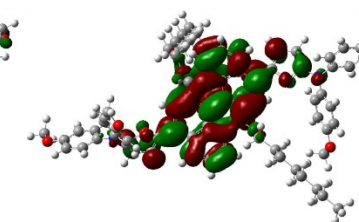
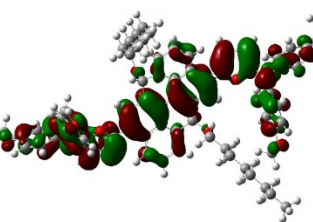
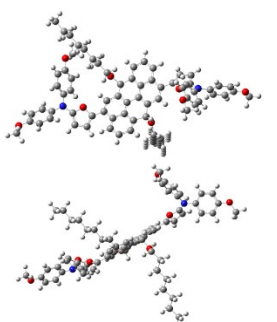
D3



D4



D5



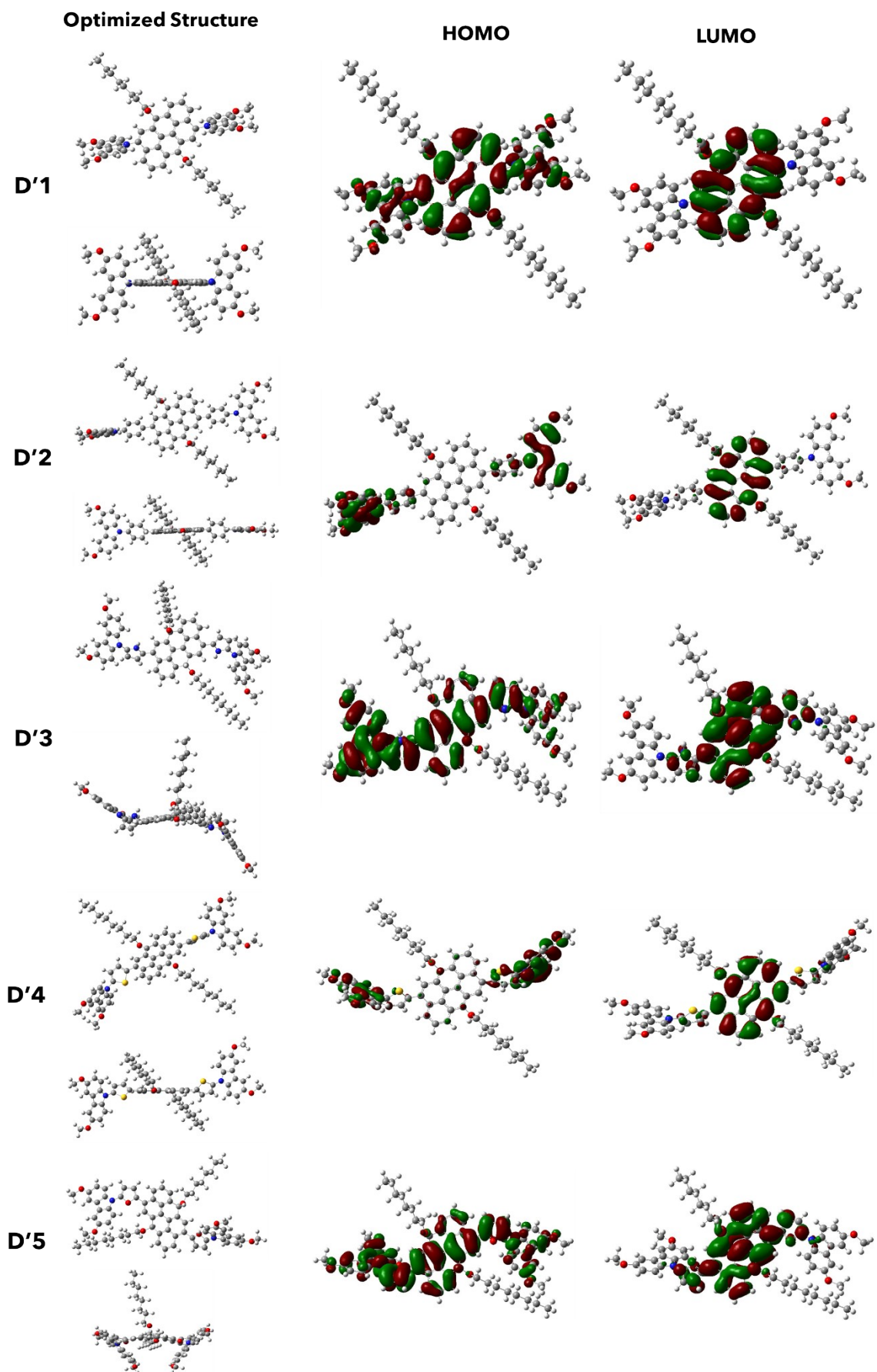


Figure S1: Optimized Structures, and HOMO-LUMO of the designed HTMs.

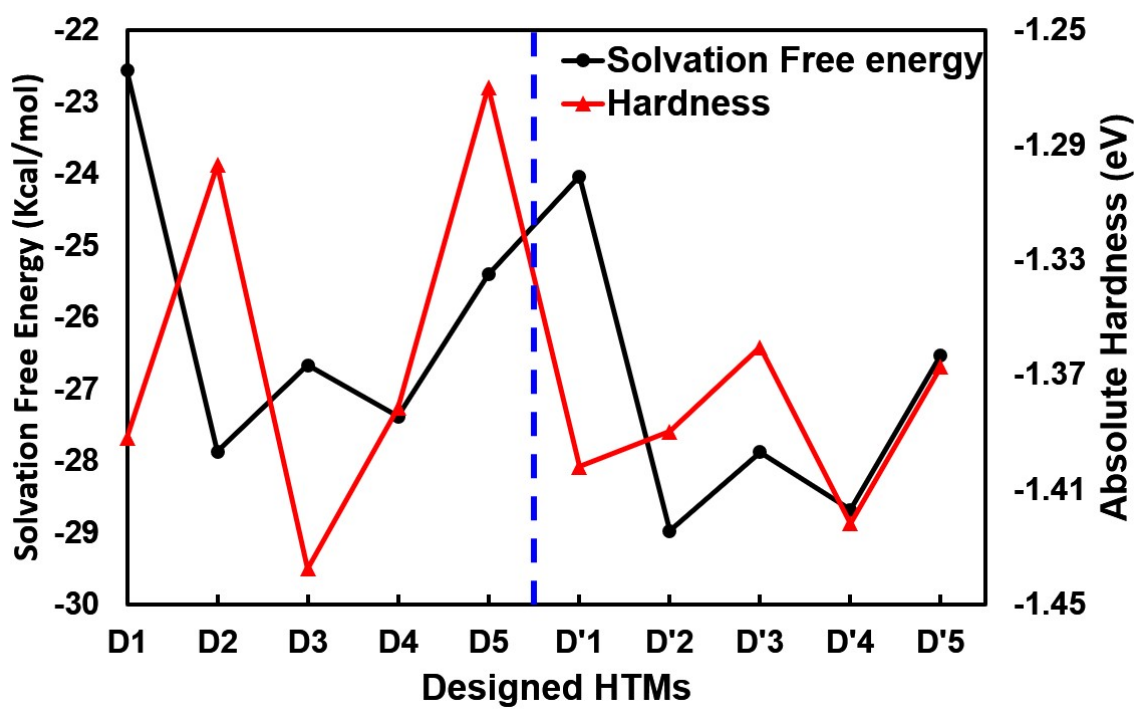


Figure S2: Chemical hardness and Solvation free energy of the designed HTMs.

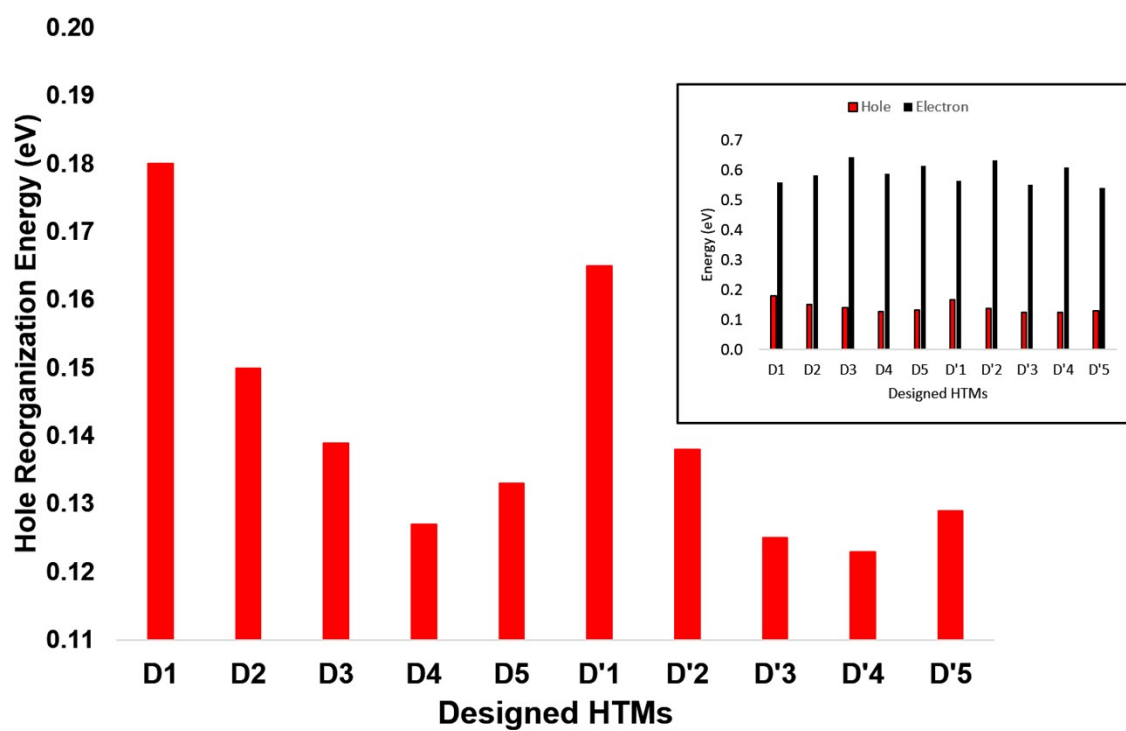


Figure S3: Hole reorganization energy of the designed HTMs. Both the hole and electron reorganization energy of the designed HTMs (inset).

Table S1: Charge transfer Integral, centroid distance, Hole hopping rate, and hole mobility of the designed HTMs.

Molecules	Pathways	Charge Integral (eV)	Centroid Distance (Å)	Hole Reorganization Energy (eV)	Hole hopping rate (S ⁻¹)	Hole Mobility (cm ² V ⁻¹ s ⁻¹)
D1	1	1.632010-03	29.36		5.8436x10 ⁹	
	2	1.905010-03	27.00		7.9622x10 ⁹	
	3	1.905010-03	28.63		7.9622x10 ⁹	
	4	6.803010-04	26.79		1.0154x10 ⁹	
	5	2.176010-03	17.84		1.0388x10 ¹⁰	
	6	1.210910-02	18.00		3.2170x10 ¹¹	
	7	2.993010-02	11.31	0.180	1.9654x10 ¹²	2.589x10 ⁻⁴
	8	1.361010-04	18.00		4.0641x10 ⁷	
D2	1	5.171010-03	43.5		5.8526x10 ¹¹	
	2	2.993310-03	43.6		1.9611x10 ¹¹	
	3	3.945610-03	46.92		3.4074x10 ¹¹	
	4	3.537510-03	46.89		2.7390x10 ¹¹	
	5	2.217710-02	19.01	0.150	1.0765x10 ¹³	4.0028x10 ⁻³
	6	7.891310-03	17.51		1.3630x10 ¹²	
	7	1.224510-02	19.43		3.2818x10 ¹²	
D3	1	1.088510-03	44.20		1.8684610x10	
	2	3.537510-03	39.58		1.9734210x11	
	3	1.278910-02	17.35	0.139	2.5792910x12	1.0948x10 ⁻³
	4	1.020410-02	20.37		1.6419810x12	
	5	4.082010-04	19.73		2.6276810x09	
	6	3.537510-03	19.52		1.9734210x11	
D4	1	7.965010-03	31.71		1.6771710x12	
	2	1.755010-03	42.28		8.1425410x10	
	3	3.510010-03	37.48		3.2570210x11	
	4	4.860010-03	32.78		6.2442210x11	
	5	8.100010-04	36.78		1.7345110x10	
	6	6.750010-04	35.86		1.2045210x10	
	7	2.295010-03	31.52		1.3924210x11	
	8	6.858010-02	15.56	0.127	1.2433710x14	3.0768x10 ⁻³
	9	3.510010-03	11.00		3.2570210x11	
	10	6.521010-02	19.62		1.1241810x14	
D5	1	1.250010-04	35.58		5.4094510x08	
	2	5.400010-03	39.36		1.0095310x12	
	3	1.920010-03	36.74		1.2762510x11	
	4	1.930010-03	39.36		1.2895810x11	
	5	1.674010-02	19.52		9.7016210x12	
	6	1.053010-02	29.58		3.8387510x12	
	7	5.413510-02	15.71	0.133	1.0145910x14	9.4314x10 ⁻²
D'1	1	5.5410-03	36.50		9.5038910x11	
	2	5.6710-03	40.57		9.9731510x11	
	3	2.1610-03	41.30		1.4473510x11	
	4	6.3510-03	36.75		1.2489110x12	

	5	6.4810-03	40.34		1.3026210x12	
	6	5.9410-03	35.45		1.0945610x12	
	7	2.3010-03	35.71		1.6339210x11	
	8	4.8610-03	40.38		7.3272110x11	
	9	8.1010-03	14.25		2.0353410x12	
	10	2.7310-02	10.51	0.165	2.3069410x13	2.6197x10 ⁻³
D'2	1	2.258610-01	40.09		2.1760510x15	
	2	1.130010-01	44.37		5.4466210x14	
	3	1.167810-01	41.76		5.8171210x14	
	4	2.637910-01	42.72		2.9684210x15	
	5	1.067910-01	44.37		4.8644010x14	
	6	1.298710-01	18.21		7.1949210x14	
	7	9.504010-02	15.08	0.138	3.8532010x14	1.4631x10 ⁻¹
	8	4.158010-02	12.61		7.3752610x13	
D'3	1	3.375010-03	38.50		2.4515410x11	
	2	3.631510-02	43.46		2.8383310x13	
	3	2.632510-02	41.31		1.4915110x13	
	4	1.363510-02	40.79		4.0013010x12	
	5	1.827910-01	43.46		7.1911010x14	
	6	1.350010-03	15.53		3.9224610x10	
	7	2.052010-02	13.52		9.0624510x12	
	8	6.480010-02	20.18		9.0373410x13	
	9	1.773910-01	15.03	0.125	6.7725010x14	2.6133x10 ⁻¹
D'4	1	8.370010-03	36.25		2.4708410x12	
	2	3.375010-03	39.04		4.0173610x11	
	3	1.215010-03	34.97		5.2065010x10	
	4	8.910010-03	37.62		2.7999410x12	
	5	6.885010-03	36.64		1.6718610x12	
	6	1.782010-02	15.08		1.1199810x13	
	7	3.064510-02	14.50	0.123	3.3121710x13	7.1727x10 ⁻³
	8	7.290010-03	20.86		1.8743410x12	
D'5	1	3.510010-02	38.42		2.9358010x13	
	2	1.552510-02	43.06		5.7434910x12	
	3	8.775010-03	15.51		1.8348810x12	
	4	2.484010-02	19.03		1.4703310x13	
	5	9.760510-02	13.90	0.129	2.2701610x14	7.5088x10 ⁻²
	6	1.066510-02	39.66		2.7104010x12	
	7	3.105010-03	36.40		2.2973910x11	
	8	3.145510-02	38.13		2.3577210x13	