Supplementary Information for the paper entitled:

Heterofission induced room temperature phosphorescence from range-separated hybrids: In search of the qualified blending components

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Full names (abbreviations) of the host and guest units under study

9H-Carbazole (Cz)

1H-Benzo[f]indole (Bd)

Dibenzo[b,d]thiophene (DBT)

Naphtho[2,3-b]thiophene (NT)

(9H-Carbazol-9-yl)(4-chlorophenyl)methanone (CPhCz)

(1H-Benzo[f]indol-1-yl)(4-chlorophenyl)methanone (CPhBd)

(4-Bromophenyl)(dibenzo[b,d]thiophen-2-yl)methanone (BrBDBT)

(4-Bromophenyl)(naphtho[2,3-b]thiophen-3-yl)methanone (BrBNT3)

9-(4,6-Diphenyl-1,3,5-triazin-2-yl)-9H-carbazole (DPhCzT)

1-(4,6-Diphenyl-1,3,5-triazin-2-yl)-1H-benzo[f]indole (DPhBdT)

Table S1. The computed values (eV) of the energy difference based on Eq. (1) using the OT-RSHs with the BLYP, PBE, and TPSS DFAs for all the combinations of the parameters α and β for the H/G systems under study.

H/G System	$\alpha = 0.0, \beta = 1.0$			$\alpha = 0.1, \beta = 0.9$		
	BLYP	PBE	TPSS	BLYP	PBE	TPSS
Cz/Bd	-1.27	-1.18	-0.96	-1.13	-1.03	-0.82
CPhCz/CPhBd	-2.08	-2.07	-2.13	-2.11	-2.10	-2.16
DPhCzT/DPhBdT	-2.66	-2.66	-2.72	-2.74	-2.74	-2.79
DBT/NT	-1.05	-0.96	-0.71	-0.90	-0.80	-0.55
BrBDBT/BrBNT3	-2.15	-2.08	-2.06	-2.15	-2.07	-2.02
	$\alpha = 0.2, \beta = 0.8$			$\alpha = 0.3, \beta = 0.7$		
	BLYP	PBE	TPSS	BLYP	PBE	TPSS
Cz/Bd	-0.93	-0.81	-0.59	-0.64	-0.49	-0.26
CPhCz/CPhBd	-2.22	-2.21	-2.26	-2.37	-2.35	-2.37
DPhCzT/DPhBdT	-2.83	-2.83	-2.63	-2.57	-2.48	-2.26
DBT/NT	-0.68	-0.56	-0.30	-0.36	-0.21	0.06
BrBDBT/BrBNT3	-2.09	-2.02	-1.90	-1.92	-1.84	-2.69
	$\alpha = 0.4, \beta = 0.6$			$\alpha = 0.5, \beta = 0.5$		
	BLYP	PBE	TPSS	BLYP	PBE	TPSS
Cz/Bd	-0.23	-0.05	0.20	0.28	0.52	0.78
CPhCz/CPhBd	-2.29	-2.16	-1.91	-1.70	-1.52	-1.24
DPhCzT/DPhBdT	-2.16	-2.02	-1.79	-1.58	-1.40	-1.14
DBT/NT	0.12	0.31	0.60	0.68	0.94	1.25
BrBDBT/BrBNT3	-1.59	-1.48	-1.23	-1.03	-0.87	-0.57

Table S2. The experimental excitation energies (eV) of the host units under study. The corresponding solvents and the values of dielectric constant are also provided.

Molecule	$E(T_1)$	$E(S_1)$	Solvent	Dielectric constant (ε)
Cz	2.25 [1,2]	3.42 [1,2]	Dichloromethane	8.93
CPhCz	2.33 [3]	2.64 [3]	Chloroform	4.71
DPhCzT	2.33 [4]	2.58 [5]	Chloroform	4.71
DBT	2.92 [6]	3.78 [6]	Ethanol	24.85
BrBDBT	2.51 [7]	3.17 [8]	1,2-Dichloroethane	10.12

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(7) K. C. Chong, C. Chen, C. Zhou, X. Chen, D. Ma, G. C. Bazan, Z. Chi and B. Liu, *Adv. Mater*., 2022, **34**, 2201569.

(8) Z. Qu, Y. Guo, J. Zhang and Z. Zhou, *Chem. Sci*., 2023, **14**, 10096-10102. (In this case, the reference data is from the CC2 approach).

Table S3. The TDA-based computed values (eV) of the energy difference based on Eq. (1) using the OT-RSHs with the BLYP, PBE, and TPSS DFAs and different combinations of the parameters α and β for the H/G systems under study.

H/G System	$\alpha = 0.0, \beta = 1.0$			$\alpha = 0.1, \beta = 0.9$		
	BLYP	PBE	TPSS	BLYP	PBE	TPSS
Cz/Bd	-1.70	-1.67	-1.60	-1.64	-1.60	-1.54
CPhCz/CPhBd	-2.09	-2.08	-2.15	-2.12	-2.11	-2.18
DPhCzT/DPhBdT	-2.66	-2.67	-2.72	-2.74	-2.74	-2.80
DBT/NT	-1.56	-1.53	-1.44	-1.49	-1.46	-1.38
BrBDBT/BrBNT3	-2.27	-2.19	-2.25	-2.32	-2.24	-2.30
	$\alpha = 0.2, \beta = 0.8$			$\alpha = 0.3, \beta = 0.7$		
	BLYP	PBE	TPSS	BLYP	PBE	TPSS
Cz/Bd	-1.55	-1.51	-1.45	-1.44	-1.39	-1.34
CPhCz/CPhBd	-2.24	-2.23	-2.29	-2.40	-2.38	-2.44
DPhCzT/DPhBdT	-2.84	-2.84	-2.89	-2.95	-2.95	-3.00
DBT/NT	-1.40	-1.37	-1.29	-1.28	-1.24	-1.17
BrBDBT/BrBNT3	-2.38	-2.30	-2.34	-2.42	-2.35	-2.38

Table S4. Statistical metrics (eV) on the performances of the proposed OT-RSHs based on the TDA with correct prediction of the relevant energetics based on Eq. (1) for the systems under study.

OT-RSHs	MSD	MAD
$\alpha = 0.0, \beta = 1.0$		
BLYP	-0.24	0.44
PBE	-0.21	0.42
TPSS	-0.21	0.46
$\alpha = 0.1, \beta = 0.9$		
BLYP	-0.25	0.47
PBE	-0.22	0.45
TPSS	-0.22	0.49
$\alpha = 0.2, \beta = 0.8$		
BLYP	-0.26	0.53
PBE	-0.23	0.51
TPSS	-0.23	0.54
$\alpha = 0.3, \beta = 0.7$		
BLYP	-0.28	0.59
PBE	-0.25	0.57
TPSS	-0.25	0.60

Table S5. The computed values of the triplet excitation energies (eV) using the PBE-based OT-RSHs with different combinations of the parameters α and β for the hosts and guests under study.

Molecule	$\alpha = 0.0, \beta = 1.0$	$\alpha = 0.1, \beta = 0.9$	$\alpha = 0.2, \beta = 0.8$	$\alpha = 0.3, \beta = 0.7$
Host				
Cz	2.64	2.57	2.48	2.35
CPhCz	2.13	2.16	2.27	2.43
DPhCzT	2.63	2.71	2.80	2.69
DBT	2.56	2.49	2.39	2.24
BrBDBT	2.24	2.27	2.27	2.23
Guest				
Bd	1.59	1.56	1.46	1.30
CPhBd	1.86	1.77	1.64	1.46
DPhBdT	1.91	1.82	1.70	1.53
NT	1.67	1.60	1.48	1.31
BrBNT3	1.86	1.78	1.67	1.51

Table S6. The computed values of the singlet excitation energies (eV) using the PBE-based OT-RSHs with different combinations of the parameters α and β for the hosts and guests under study.

Molecule	$\alpha = 0.0, \beta = 1.0$	$\alpha = 0.1, \beta = 0.9$	$\alpha = 0.2, \beta = 0.8$	$\alpha = 0.3, \beta = 0.7$
Host				
Cz	4.10	4.12	4.15	4.21
CPhCz	2.19	2.22	2.34	2.51
DPhCzT	2.59	2.67	2.78	2.90
DBT	4.16	4.18	4.21	4.27
BrBDBT	2.41	2.46	2.53	2.62
Guest				
Bd	3.58	3.56	3.57	3.60
CPhBd	1.98	2.01	2.10	2.21
DPhBdT	2.49	2.53	2.59	2.67
NT	3.62	3.62	3.63	3.66
BrBNT3	2.57	2.63	2.70	2.80

Table S7. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the singlet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.0, \beta = 1.0$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	4.10	0.44	-24.20	0.46	L
CPhCz	2.19	3.17	1.23	3.89	CT
DPhCzT	2.59	4.42	2.16	4.86	CT
DBT	4.16	0.83	-8.91	0.88	L
BrBDBT	2.41	2.08	-0.28	4.68	CT

Table S8. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.0, \beta = 1.0$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	2.64	0.02	-599.95	0.10	L
CPhCz	2.13	2.92	1.01	3.83	CT
DPhCzT	2.63	4.27	2.20	4.79	CT
DBT	2.56	0.03	-571.78	0.15	L
BrBDBT	2.24	0.91	-8.36	2.64	CT

Table S9. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the guest units computed using the PBE-based OT-RSH ($\alpha = 0.0, \beta = 1.0$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Bd	1.59	0.01	-1832.39	0.39	L
CPhBd	1.86	0.13	-107.12	1.94	L
DPhBdT	1.91	0.07	-215.85	1.82	CT
NT	1.67	0.07	-196.19	0.44	L
BrBNT3	1.86	0.31	-40.32	2.54	CT

Table S10. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the singlet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.1, \beta = 0.9$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	4.12	0.45	-23.94	0.45	L
CPhCz	2.22	3.24	1.24	3.92	CT
DPhCzT	2.67	4.47	2.22	4.88	CT
DBT	4.18	0.85	-8.67	0.88	L
BrBDBT	2.46	2.09	-0.12	4.73	CT

Table S11. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.1, \beta = 0.9$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	2.57	0.03	-488.94	0.10	L
CPhCz	2.16	2.99	1.05	3.86	CT
DPhCzT	2.71	5.67	2.58	5.78	CT
DBT	2.49	0.03	-495.65	0.16	L
BrBDBT	2.27	0.85	-9.41	2.37	CT

Table S12. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the guest units computed using the PBE-based OT-RSH ($\alpha = 0.1, \beta = 0.9$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Bd	1.56	0.01	-1142.63	0.39	L
CPhBd	1.77	0.13	-105.17	1.93	L
DPhBdT	1.82	0.07	-189.44	1.87	L
NT	1.60	0.06	-227.06	0.44	L
BrBNT3	1.78	0.28	-44.56	2.51	CT

Table S13. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the singlet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.2, \beta = 0.8$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	4.15	0.45	-24.07	0.45	L
CPhCz	2.34	3.27	1.38	3.95	CT
DPhCzT	2.78	4.52	2.31	4.92	CT
DBT	4.21	0.85	-8.64	0.88	L
BrBDBT	2.53	2.10	0.06	4.83	CT

Table S14. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.2, \beta = 0.8$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	2.48	0.04	-377.99	0.11	L
CPhCz	2.27	2.98	1.19	3.84	CT
DPhCzT	2.80	3.76	2.18	4.04	CT
DBT	2.39	0.03	-436.02	0.17	L
BrBDBT	2.27	0.74	-11.69	1.96	L

Table S15. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the guest units computed using the PBE-based OT-RSH ($\alpha = 0.2, \beta = 0.8$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Bd	1.46	0.03	-519.03	0.38	L
CPhBd	1.64	0.14	-95.84	2.03	CT
DPhBdT	1.70	0.08	-169.40	1.97	L
NT	1.48	0.06	-236.37	0.43	L
BrBNT3	1.67	0.24	-51.82	2.48	CT

Table S16. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the singlet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.3, \beta = 0.7$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	4.21	0.44	-24.72	0.44	L
CPhCz	2.51	3.27	1.61	3.96	CT
DPhCzT	2.90	4.58	2.39	4.95	CT
DBT	4.27	0.84	-8.82	0.87	L
BrBDBT	2.62	2.82	0.25	4.96	CT

Table S17. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.3, \beta = 0.7$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	2.35	0.05	-307.90	0.11	L
CPhCz	2.43	2.91	1.41	3.79	CT
DPhCzT	2.69	0.01	-1020.51	0.71	L
DBT	2.24	0.03	-454.69	0.18	L
BrBDBT	2.23	0.55	-17.85	2.39	CT

Table S18. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the guest units computed using the PBE-based OT-RSH ($\alpha = 0.3, \beta = 0.7$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Bd	1.30	0.05	-282.36	0.39	L
CPhBd	1.46	0.08	-177.79	2.07	CT
DPhBdT	1.53	0.08	-168.14	2.06	CT
NT	1.31	0.05	-286.52	0.43	L
BrBNT3	1.51	0.22	-58.97	2.51	CT

Table S19. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the singlet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.4, \beta = 0.6$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	4.28	0.43	-25.51	0.44	L
CPhCz	2.61	3.46	1.67	3.91	CT
DPhCzT	3.04	4.63	2.46	4.98	CT
DBT	4.36	0.81	-9.30	0.86	L
BrBDBT	2.71	2.06	0.45	5.05	CT

Table S20. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.4, \beta = 0.6$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	2.16	0.05	-260.90	0.12	L
CPhCz	2.39	0.72	-11.16	1.77	L
DPhCzT	2.53	0.04	-316.81	0.72	L
DBT	2.03	0.04	-346.94	0.20	L
BrBDBT	2.10	0.43	-25.10	2.44	CT

Table S21. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the guest units computed using the PBE-based OT-RSH ($\alpha = 0.4, \beta = 0.6$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Bd	1.03	0.07	-191.50	0.39	L
CPhBd	1.21	0.13	-107.30	2.12	CT
DPhBdT	1.28	0.08	-179.08	2.12	CT
NT	1.00	0.04	-384.28	0.42	L
BrBNT3	1.27	0.16	-80.89	2.50	CT

Table S22. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the singlet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.5, \beta = 0.5$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	4.36	0.39	-28.78	0.43	L
CPhCz	2.78	3.32	1.78	4.02	CT
DPhCzT	3.23	4.68	2.52	5.01	CT
DBT	4.44	0.79	-9.85	0.84	L
BrBDBT	2.86	1.93	0.64	4.67	CT

Table S23. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the host units computed using the PBE-based OT-RSH ($\alpha = 0.5, \beta = 0.5$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Cz	1.92	0.06	-218.96	0.13	L
CPhCz	2.15	0.08	-163.26	1.17	L
DPhCzT	2.32	0.06	-229.04	0.80	L
DBT	1.75	0.04	-330.30	0.22	L
BrBDBT	1.86	0.32	-34.73	2.32	CT

Table S24. The excitation energies, values of D, M_{AC}, and $\Delta\mathbf{r}$ indexes as well as the character of the triplet excited states of the guest units computed using the PBE-based OT-RSH ($\alpha = 0.5, \beta = 0.5$).

Molecule	$E(eV)$	$D(\text{Å})$	$M_{AC}(eV)$	Δr (Å)	Character
Bd	0.58	0.07	-198.70	0.39	L
CPhBd	0.78	0.06	-215.95	2.19	CT
DPhBdT	0.86	0.06	-220.78	2.23	CT
NT	0.50	0.03	-560.73	0.41	L
BrBNT3	0.89	0.16	-80.60	2.45	CT

Table S25. The computed values (eV) of the energy difference based on Eq. (1) using the PBE-based OT-RSH ($\alpha = 0.0, \beta = 1.0$) with different basis sets for the H/G systems under study. Also given as the boldface in the last rows are the corresponding statistical metrics against the reference data obtained from Table S2.

H/G System	6-31+G(d)	6-311++G(d,p)	6-311++G(2df,2p)	TZVP
Cz/Bd	-1.18	-1.16	-1.15	-1.15
CPhCz/CPhBd	-2.07	-2.08	-2.09	-2.09
DPhCzT/DPhBdT	-2.66	-2.66	-2.68	-2.67
DBT/NT	-0.96	-0.98	-0.99	-0.97
BrBDBT/BrBNT3	-2.08	-2.07	-2.06	-2.06
MSD	**0.03**	**0.03**	**0.02**	**0.03**
MAD	**0.41**	**0.41**	**0.41**	**0.40**

Table S26. The computed values (eV) of the energy difference based on Eq. (1) using the PBE-based OT-RSH ($\alpha = 0.0, \beta = 1.0$) with different integration grids for the H/G systems under study. Also given as the boldface in the last rows are the corresponding statistical metrics against the reference data obtained from Table S2.

H/G System	*FineGrid*	*UltraFineGrid*	*SuperFineGrid*
Cz/Bd	-1.18	-1.18	-1.18
CPhCz/CPhBd	-2.07	-2.07	-2.07
DPhCzT/DPhBdT	-2.66	-2.66	-2.66
DBT/NT	-0.96	-0.96	-0.96
BrBDBT/BrBNT3	-2.08	-2.08	-2.08
MSD	**0.03**	**0.03**	**0.03**
MAD	**0.41**	**0.41**	**0.41**

Table S27. The computed values (eV) of the energy difference based on Eq. (1) for the H/G systems under study using the PBE-based OT-RSH ($\alpha = 0.0, \beta = 1.0$) and their standard versions within the frameworks of LR-PCM (eq), LR-PCM (non-eq), SS-PCM (eq), and SS-PCM (non-eq).

H/G systems		LR-PCM (non-eq)		LR-PCM (eq)		SS-PCM (non-eq)		SS-PCM (eq)	
OT-RSH	LC-PBE	OT-RSH	LC-PBE	OT-RSH	LC-PBE	OT-RSH	LC-PBE		
Cz/Bd		-1.90	0.69	-1.93	0.66	-1.89	0.72	-1.91	0.72
CPhCz/CPhBd		-1.37	-0.94	-1.37	-0.94	-1.07	-1.11	-0.90	-1.20
DPhCzT/DPhBdT		-1.81	-0.25	-1.81	-0.25	-1.49	-0.29	-1.31	-0.30
DBT/NT		-1.74	1.28	-1.77	1.24	-1.74	1.28	-1.77	1.24
BrBDBT/BrBNT3		-2.33	-1.04	-2.33	-1.04	-2.33	-1.04	-2.33	-1.04

Table S28. Optimally tuned values of the range-separation parameter for the theoretically designed host and guest units. All values are in $Bohr^{-1}$.

Molecule	μ
I	0.1968
II	0.1996
III	0.2150
IV	0.2033
V	0.2503
VI	0.2097
VII	0.2259
VIII	0.2000

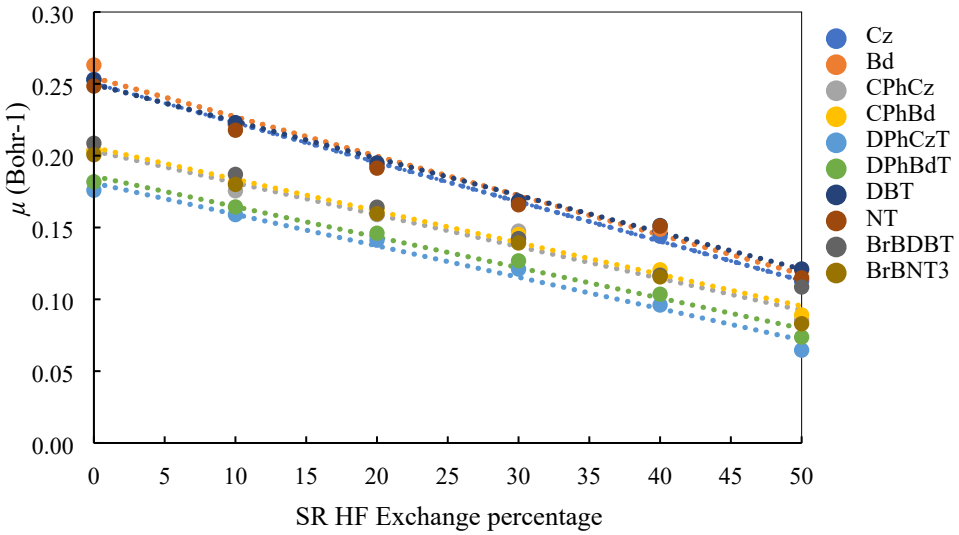

Figure S1. Correlation between the optimally tuned values of the range-separation parameter (Bohr^{-1}) and the HF exchange contribution at the short-range regime for all the considered host and guest units.

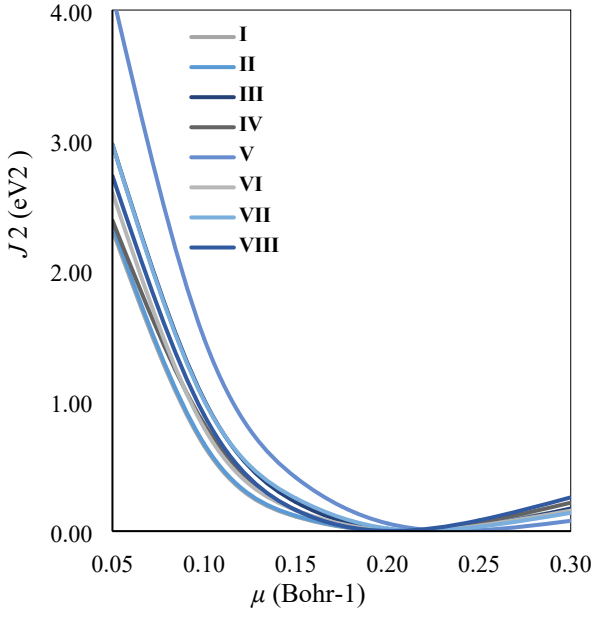

Figure S2. Plot of the target function J^2 versus the range-separation parameter μ for the theoretically designed host and guest units.