Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for the paper entitled:

Excited-States Properties of Organic Semiconductor Dyes as Electrically Pumped Lasing Candidates from New Optimally Tuned Range-Separated Models

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This file includes 11 tables (Tables S1-S11) and 2 figures (Figures S1 and S2).

Table S1. Computed values (eV) of the emission energies of the systems under study using the proposed OT-RSHs based on different DFAs, *i.e.*, BLYP, PBE, and TPSS, for the $\alpha = 0.0, \beta = 1.0$ combination. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP	PBE	TPSS
BP3T	2.17 [a]	2.44	2.47	2.48
BSBCz	2.58 [b]	2.85	2.87	2.90
CzPVSBF	2.63 [c]	2.79	2.80	2.83
BPBFCz1	2.56 [d]	2.99	3.00	3.03
BPBFCz2	2.90 [d]	3.07	3.08	3.11
MSD		**0.26**	**0.28**	**0.30**
MAD		**0.26**	**0.28**	**0.30**
RMSD		**0.28**	**0.29**	**0.32**

[a] M. Ichikawa, K. Nakamura, M. Inoue, H. Mishima, T. Haritani, R. Hibino, T. Koyama and Y. Taniguchi, *Appl. Phys. Lett.*, 2005, **87**, 221113-1-221113-3.

[b] A. S. D. Sandanayaka, K. Yoshida, M. Inoue, C. Qin, K. Goushi, J.-C. Ribierre, T. Matsushima and C. Adachi, *Adv. Opt. Mater.* 2016, **4**, 834-839.

[c] H. Nakanotani, S. Akiyama, D. Ohnishi, M. Moriwake, M. Yahiro, T. Yoshihara, S. Tobita and C. Adachi, *Adv. Funct. Mater*. **2007**, *17*, 2328-2335.

[d] Y. Oyama, M. Mamada, A. Shukla, E. G. Moore, S.-C. Lo, E. B. Namdas and C. Adachi, *ACS Mater. Lett*. 2020, **2**, 161-167.

Note: How to obtain the experimental data for each organic semiconductor dye is briefly as follows: BP3T[a] (electroluminescence spectrum of a single crystal, where vibronic progression peak was used to determine the maximum wavelength); BSBCz[b] (emission spectrum measured from the laser device of neat films at different excitation intensities); CzPVSBF[c] (photoluminescence spectrum in neat film, corresponds to the amplified-spontaneous-emission (ASE) peak wavelength); BPBFCz1[d] and BPBFCz2[d] (photoluminescence spectra in neat films).

Table S2. Computed values (eV) of the emission energies of the systems under study using the proposed OT-RSHs based on different DFAs, *i.e.*, BLYP, PBE, and TPSS, for the $\alpha = 0.1, \beta = 0.9$ combination. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP	PBE	TPSS
BP3T	2.17	2.40	2.43	2.45
BSBCz	2.58	2.72	2.75	2.78
CzPVSBF	2.63	2.68	2.69	2.73
BPBFCz1	2.56	2.94	2.96	2.99
BPBFCz2	2.90	3.01	3.02	3.05
MSD		**0.18**	**0.20**	**0.23**
MAD		**0.18**	**0.20**	**0.23**
RMSD		**0.22**	**0.23**	**0.26**

Table S3. Computed values (eV) of the emission energies of the systems under study using the proposed OT-RSHs based on different DFAs, *i.e.*, BLYP, PBE, and TPSS, for the $\alpha = 0.2, \beta = 0.8$ combination. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP	PBE	TPSS
BP3T	2.17	2.35	2.38	2.40
BSBCz	2.58	2.72	2.73	2.77
CzPVSBF	2.63	2.61	2.62	2.66
BPBFCz1	2.56	2.87	2.88	2.91
BPBFCz2	2.90	2.93	2.95	2.98
MSD		**0.13**	**0.14**	**0.18**
MAD		**0.14**	**0.15**	**0.18**
RMSD		**0.17**	**0.19**	**0.21**

Table S4. Computed values (eV) of the emission energies of the systems under study using the proposed OT-RSHs based on different DFAs, *i.e.*, BLYP, PBE, and TPSS, for the $\alpha = 0.3, \beta = 0.7$ combination. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP	PBE	TPSS
BP3T	2.17	2.30	2.32	2.34
BSBCz	2.58	2.64	2.65	2.69
CzPVSBF	2.63	2.51	2.52	2.56
BPBFCz1	2.56	2.75	2.76	2.80
BPBFCz2	2.90	2.85	2.87	2.91
MSD		**0.04**	**0.06**	**0.09**
MAD		**0.11**	**0.11**	**0.12**
RMSD		**0.12**	**0.13**	**0.14**

Table S5. Computed values (eV) of the emission energies of the systems under study using the proposed OT-RSHs based on different DFAs, *i.e.*, BLYP, PBE, and TPSS, for the $\alpha = 0.4, \beta = 0.6$ combination. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP	PBE	TPSS
BP3T	2.17	2.22	2.24	2.26
BSBCz	2.58	2.51	2.52	2.56
CzPVSBF	2.63	2.37	2.38	2.43
BPBFCz1	2.56	2.59	2.60	2.65
BPBFCz2	2.90	2.73	2.74	2.79
MSD		**-0.08**	**-0.07**	**-0.03**
MAD		**0.12**	**0.12**	**0.10**
RMSD		**0.14**	**0.14**	**0.12**

Table S6. The computed values (eV) of the emission energies of the systems under study using the best proposed OT-RSHs in this work and 6-31+G(d) basis set. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP ($\alpha = 0.3, \beta = 0.7$)	PBE ($\alpha = 0.3, \beta = 0.7$)	TPSS ($\alpha = 0.4, \beta = 0.6$)
BP3T	2.17	2.21	2.26	2.20
BSBCz	2.58	2.58	2.60	2.51
CzPVSBF	2.63	2.46	2.48	2.39
BPBFCz1	2.56	2.70	2.72	2.62
BPBFCz2	2.90	2.80	2.83	2.75
MSD		**-0.02**	**0.01**	**-0.07**
MAD		**0.09**	**0.10**	**0.11**
RMSD		**0.11**	**0.11**	**0.13**

Table S7. The computed values (eV) of the emission energies of the systems under study using the best proposed OT-RSHs in this work and 6-311G(d,p) basis set. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP ($\alpha = 0.3, \beta = 0.7$)	PBE ($\alpha = 0.3, \beta = 0.7$)	TPSS ($\alpha = 0.4, \beta = 0.6$)
BP3T	2.17	2.25	2.28	2.23
BSBCz	2.58	2.59	2.61	2.52
CzPVSBF	2.63	2.47	2.48	2.40
BPBFCz1	2.56	2.70	2.72	2.61
BPBFCz2	2.90	2.81	2.83	2.75
MSD		**0.00**	**0.02**	**-0.07**
MAD		**0.10**	**0.10**	**0.11**
RMSD		**0.11**	**0.11**	**0.13**

Table S8. The computed values (eV) of the emission energies of the systems under study using the best proposed OT-RSHs in this work and 6-311++G(d,p) basis set. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP ($\alpha = 0.3, \beta = 0.7$)	PBE ($\alpha = 0.3, \beta = 0.7$)	TPSS ($\alpha = 0.4, \beta = 0.6$)
BP3T	2.17	2.20	2.25	2.19
BSBCz	2.58	2.56	2.58	2.50
CzPVSBF	2.63	2.44	2.46	2.38
BPBFCz1	2.56	2.68	2.70	2.60
BPBFCz2	2.90	2.78	2.80	2.73
MSD		**-0.04**	**-0.01**	**-0.09**
MAD		**0.10**	**0.10**	**0.11**
RMSD		**0.11**	**0.11**	**0.14**

Table S9. The computed values of the emission oscillator strengths of the systems under study using the best proposed OT-RSHs in this work.

Molecule	BLYP ($\alpha = 0.3, \beta = 0.7$)	PBE ($\alpha = 0.3, \beta = 0.7$)	TPSS ($\alpha = 0.4, \beta = 0.6$)
BP3T	2.38	2.41	2.45
BSBCz	3.29	3.30	3.15
CzPVSBF	2.99	3.01	2.83
BPBFCz1	2.53	2.52	2.26
BPBFCz2	2.83	2.85	2.74

Table S10. The computed values (eV) of the emission energies of the systems under study using the best proposed OT-RSHs-PCM in this work. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP ($\alpha = 0.3, \beta = 0.7$)	PBE ($\alpha = 0.3, \beta = 0.7$)	TPSS ($\alpha = 0.4, \beta = 0.6$)
BP3T	2.17	2.17	2.20	2.14
BSBCz	2.58	2.57	2.58	2.49
CzPVSBF	2.63	2.44	2.45	2.36
BPBFCz1	2.56	2.69	2.70	2.61
BPBFCz2	2.90	2.79	2.80	2.72

Table S11. The computed values (eV) of the emission energies of the systems under study using the best proposed OT-SRSHs in this work. Also given in the table are the experimental data used as reference (Ref.). The corresponding statistical metrics are shown in boldface.

Molecules	Ref.	BLYP ($\alpha = 0.3, \beta = 0.7$)	PBE ($\alpha = 0.3, \beta = 0.7$)	TPSS ($\alpha = 0.4, \beta = 0.6$)
BP3T	2.17	2.02	2.04	2.03
BSBCz	2.58	2.28	2.28	2.26
CzPVSBF	2.63	2.20	2.20	2.18
BPBFCz1	2.56	2.37	2.37	2.34
BPBFCz2	2.90	2.50	2.52	2.50

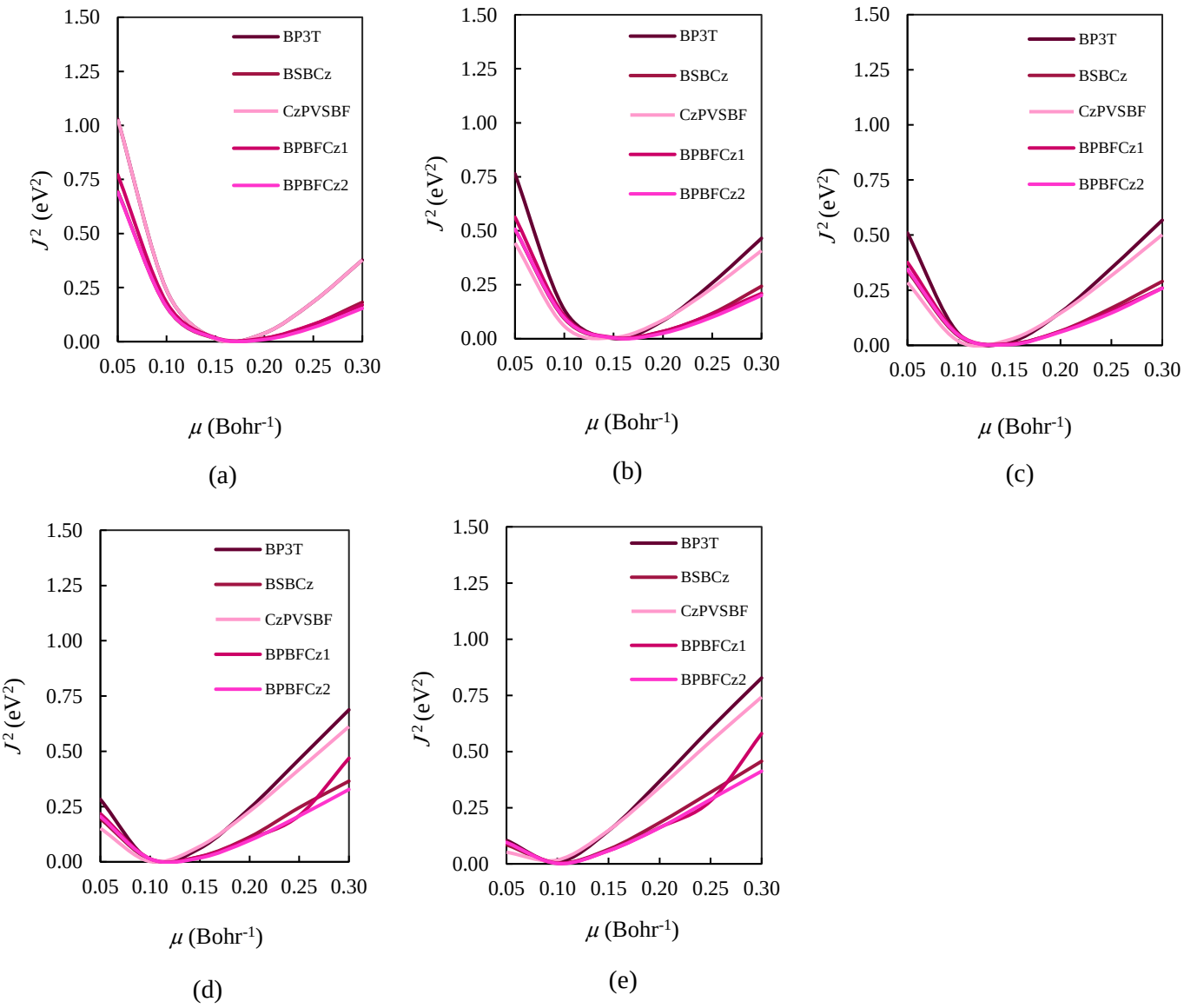

Figure S1. Plots of the target function J^2 versus the range-separation parameter μ for the systems under study. (a) $\alpha = 0.0, \beta = 1.0$, (b) $\alpha = 0.1, \beta = 0.9$, (c) $\alpha = 0.2, \beta = 0.8$, (d) $\alpha = 0.3, \beta = 0.7$, and (e) $\alpha = 0.4, \beta = 0.6$.

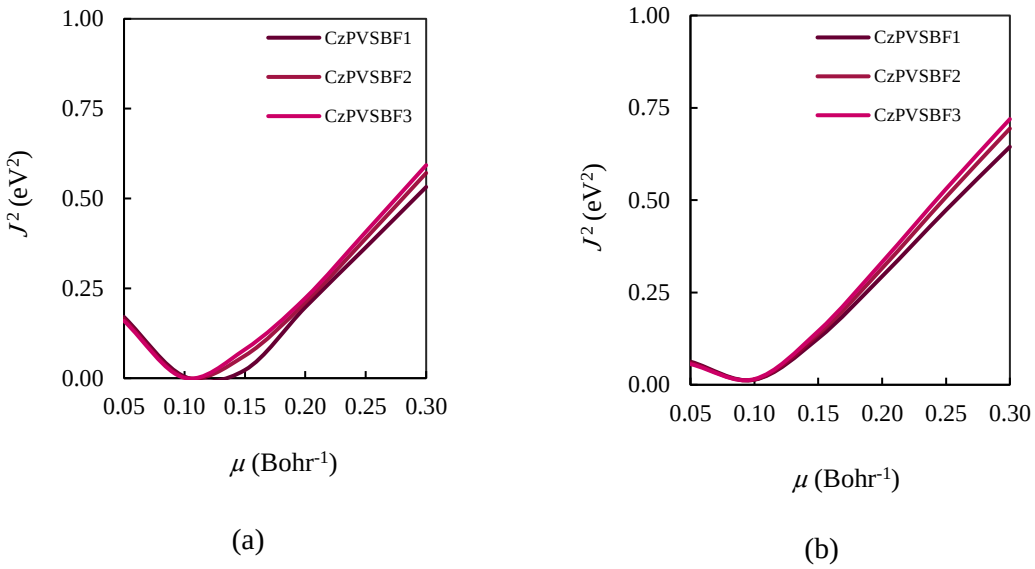

Figure S2. Plots of the target function J^2 versus the range-separation parameter μ for the theoretically designed chromophores in this work. (a) $\alpha = 0.3, \beta = 0.7$ and (b) $\alpha = 0.4, \beta = 0.6$.