

Supporting Information

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Triarylborane functionalized selenophenothiophene analogues: syntheses, photophysical and electrochemical properties

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Computation

Absorption Spectra

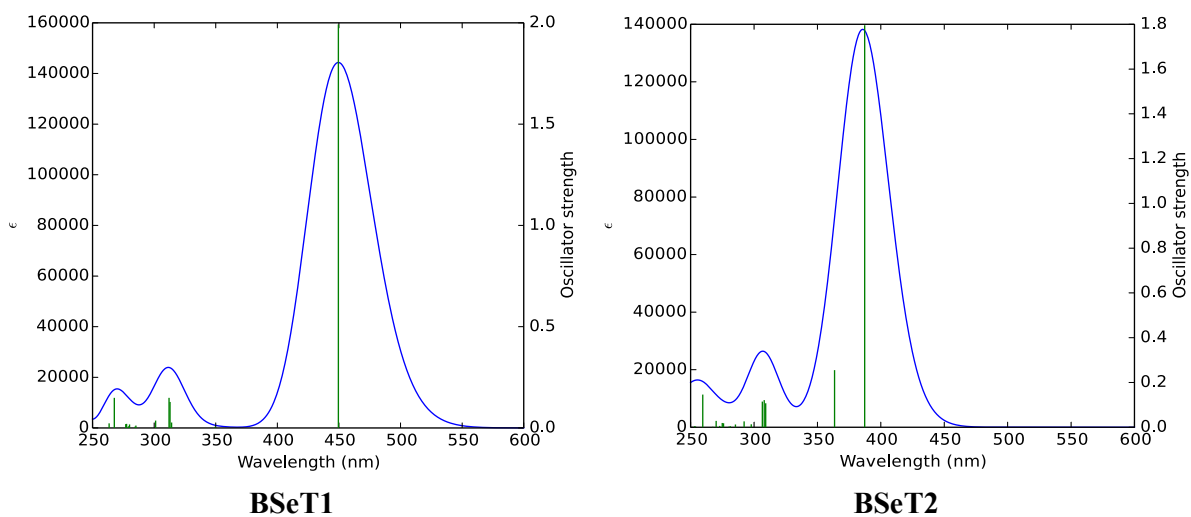


Figure S5. Absorption spectra predicted at (PCM:THF)-CAM-TD-B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level.

Cartesian Coordinates

BSeT1

C -0.1770500 0.5185170 0.0450860
C 0.3207350 -0.7836650 0.0779770
S 1.1272440 1.6778230 0.0182920
Se -1.0842130 -2.0198540 0.0996630
B 7.7640950 0.1595680 -0.0201040
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