

Photoluminescence of Cis-Polyacetylene Semiconductor Material

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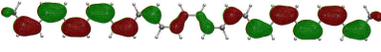
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Table S1.: Hole and electron NTOs of the complex OLIG. All NTOs are Calculated using TDDFT on the ground state geometry with PBE functional and LANL2dz/6-31G* basis set with dichloromethane solvent using CPCM method.

OLIG	Hole	Electron
S ₁ E = 1.90 eV <i>f</i> =3.7777		
S ₄ E = 2.67 eV <i>f</i> =0.4562		
S ₈ E = 3.23 eV <i>f</i> =0.2856		
S ₁₀ E = 3.64 eV <i>f</i> =0.0227 H/L : 64%		
S ₁₁ E = 3.71 eV <i>f</i> =0.4216		

<p>S₁₄ E = 3.88 eV <i>f</i>=0.1393 H/L : 39%</p>		
<p>S₁₉ E = 4.41 eV <i>f</i>=0.0807 H/L : 33%</p>		
<p>S₂₄ E = 4.79 eV <i>f</i>=0.2097</p>	