

Photoluminescence of Cis-Polyacetylene Semiconductor Material

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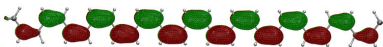

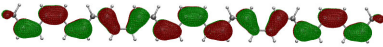
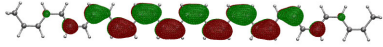


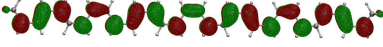
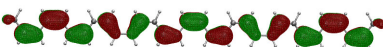

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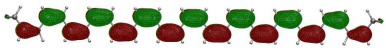
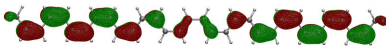
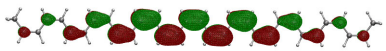

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Table S1.: Hole and electron NTOs of the complex OLIG. All NTOs are Calculated using TDDFT on the ground state geometry with PBE functional and LANL2dz/6-31G* basis set with dichloromethane solvent using CPCM method.

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