Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Information

On the nature of the photochemical reaction of polypyridyl Ru(II) complexes leading to sunlight-to-chemical energy conversion: Density functional analysis

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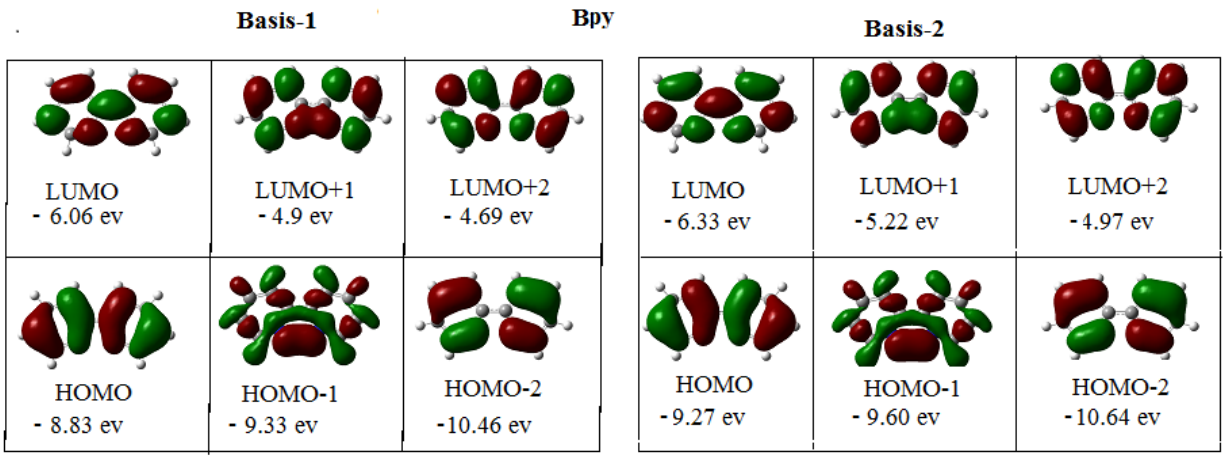


Figure S1. (a) Comparison of the MO shapes and energies of an isolated bpy molecule in acetonitrile determined from the DFT calculations with Basis-1 and Basis-2.

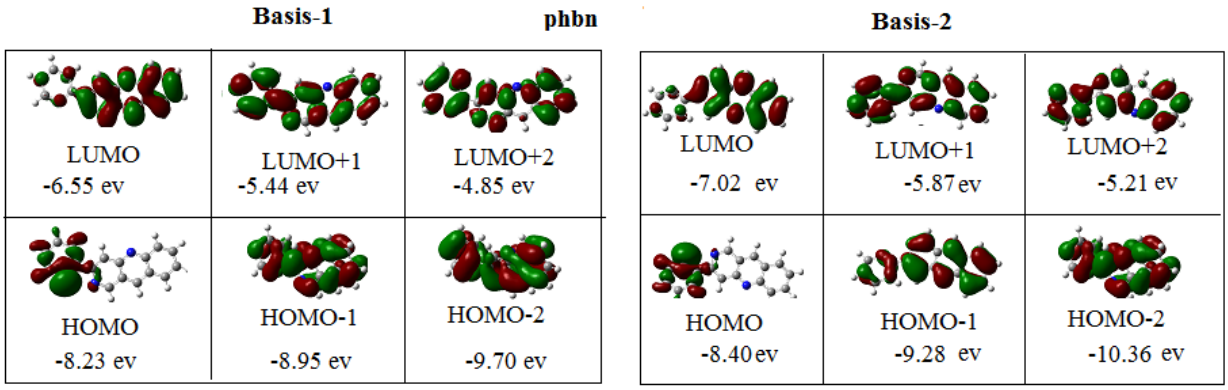


Figure S1. (b) Comparison of the MO shapes and energies of an isolated $phbn^-$ anion in acetonitrile determined from the DFT calculations with Basis-1 and Basis-2.

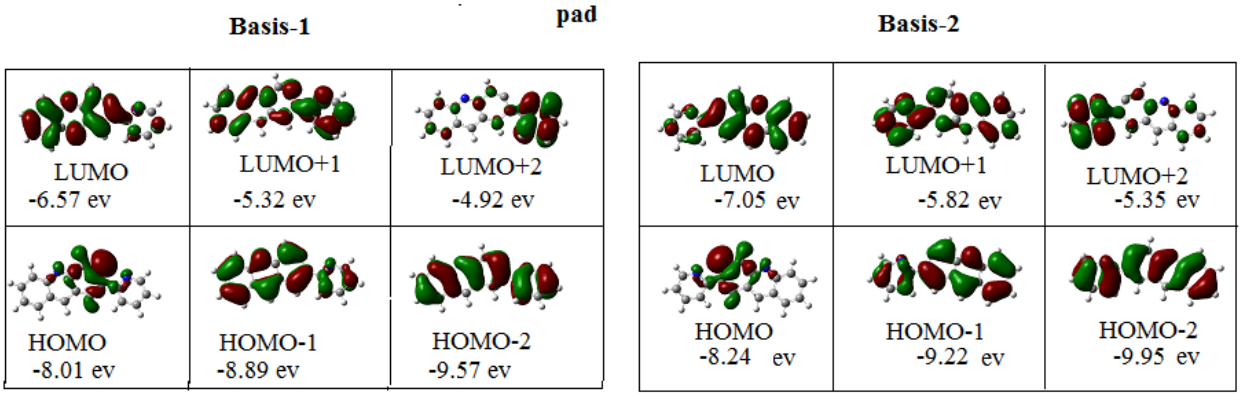


Figure S1. (c) Comparison of the MO shapes and energies of isolated pad^{-} anion in acetonitrile determined from the DFT calculations with Basis-1 and Basis-2

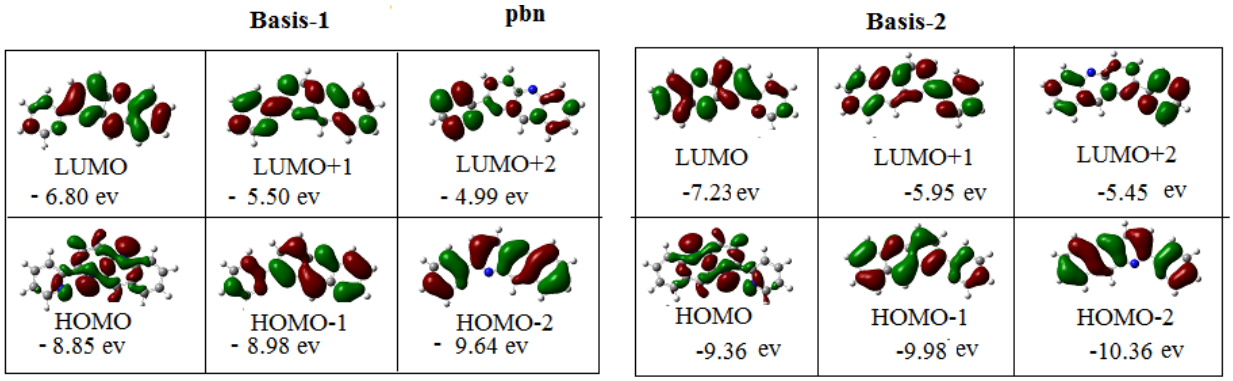


Figure S1. (d) Comparison of the MO shapes and energies of an isolated pbn^{0} molecule in acetonitrile determined from the DFT calculations with Basis-1 and Basis-2.

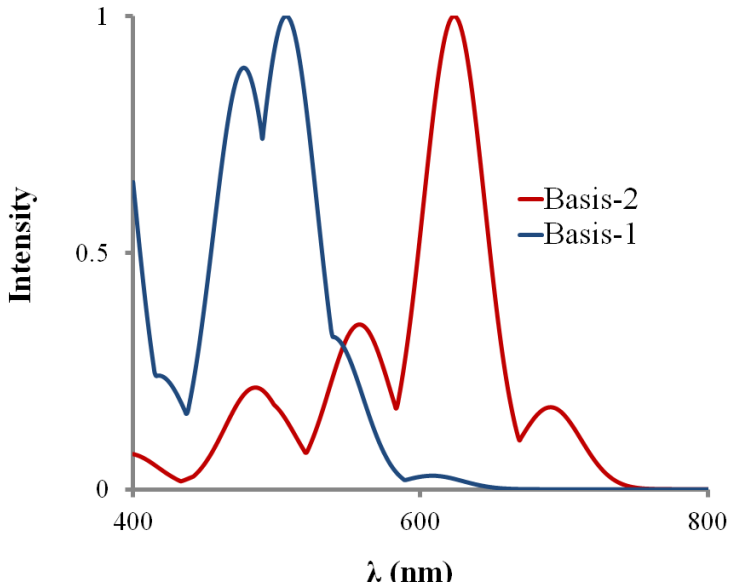
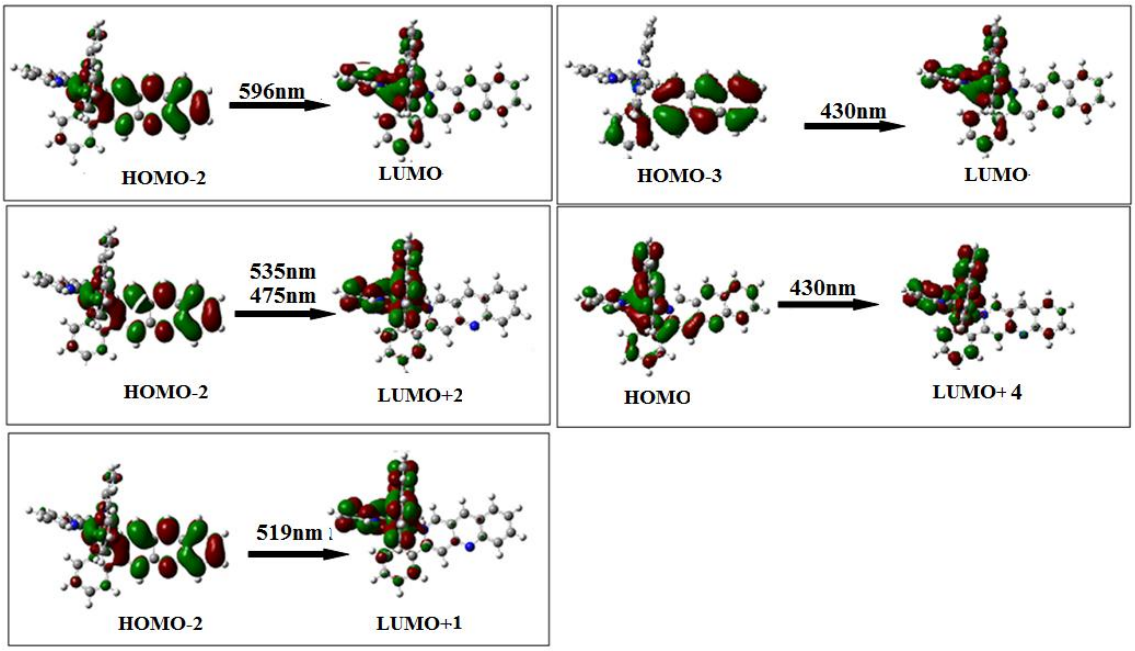
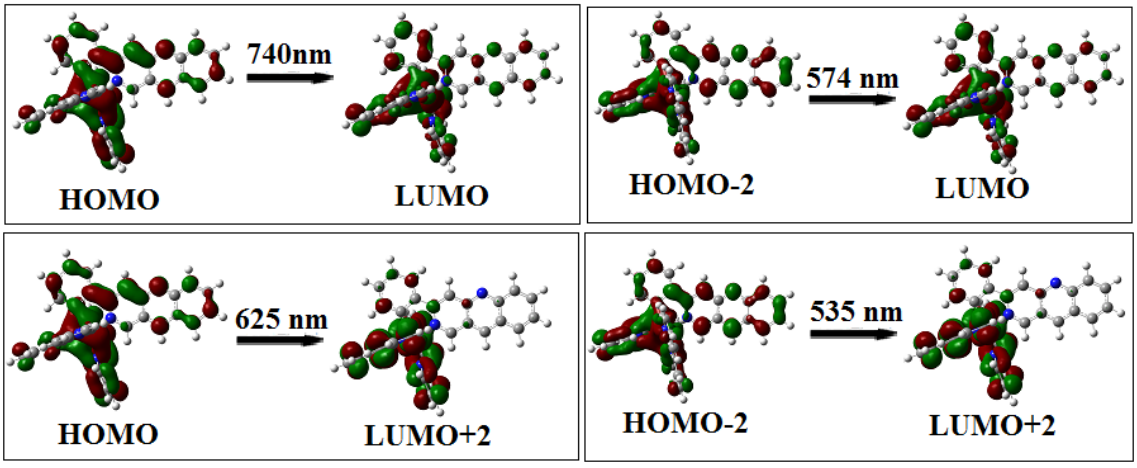


Figure S2. The comparison of the absorption spectra of the Ru (II) complexe **2** obtained from the TD-DFT calculations with (a) Basis-1 and (b) Basis-2. The intensities of the calculated absorption peaks were scaled with respect to the strongest one in the visible region, which was assigned to have the intensity of 1.0.



(a)



(b)

Figure S3. The molecular orbitals involved in the optical absorption of **1** (with **L** = **phbn**) in the visible region obtained from the TD-DFT calculations with (a) Basis-1 and (b) Basis-2.

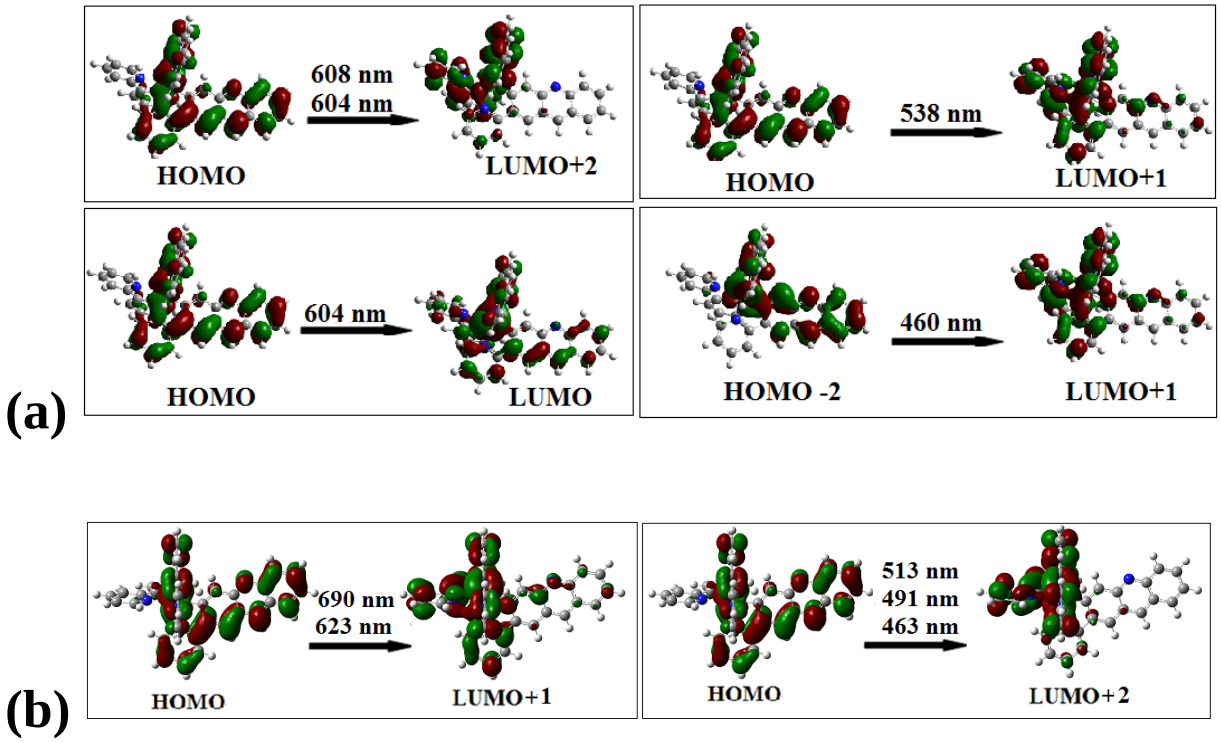


Figure S4. The molecular orbitals involved in the optical absorption of **2** in the visible region from the TD-DFT calculations with Basis-1 in (a), and those with Basis-2 in (b).