Electronic Supplementary Information (ESI)

Gold nanocomposite assemblies using functionalized Ru(II)-polypyridyl complexes

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Fig. S1 Mass profile of $Ru(2,2'\text{-bpy})_2(4\text{-ATP})_2.2PF_6$ complex (I)

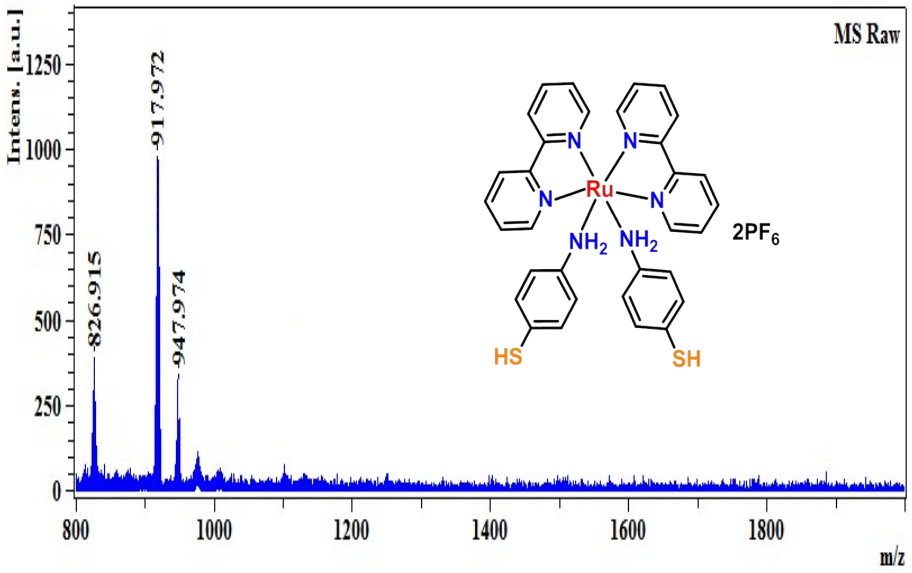


Fig. S2 FT-IR spectral bands of $Ru(1,10\text{-phen})_2(4\text{-ATP})_2.2PF_6$ complex (II)

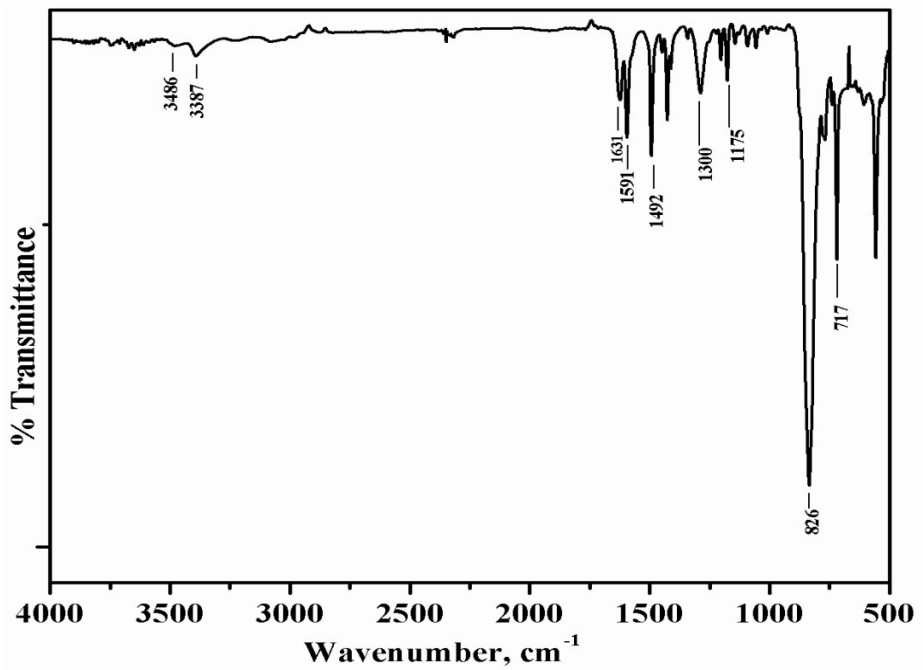


Fig. S3 Additional HRTEM images, SAED and FFT pattern of surface functionalized Au-Ru(II)polypyridyl nanocomposites by $Ru(II)(2,2'\text{-bpy})_2(4\text{-ATP})_2.2PF_6$ molecule (I).

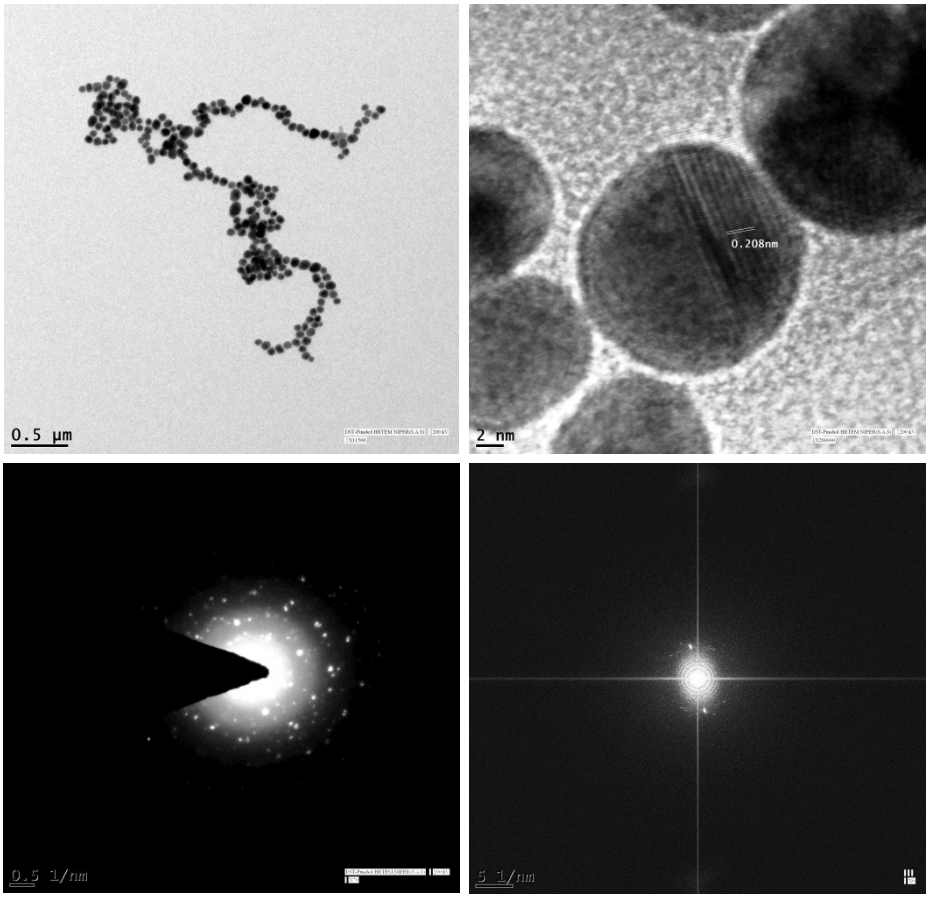
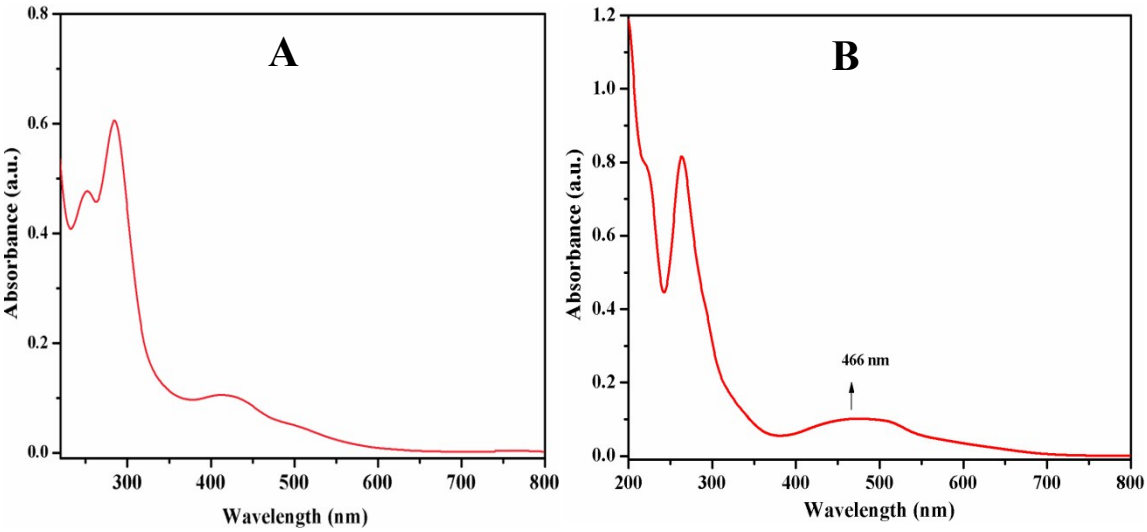
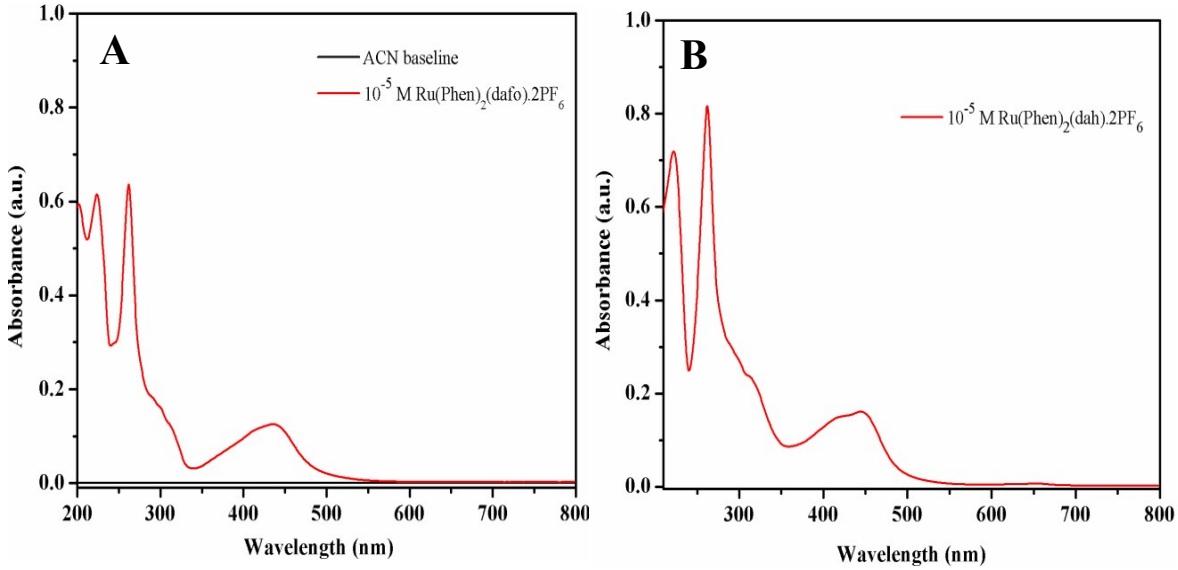


Fig. S4 UV-vis spectra of, (A) 10^{-5} M Ru(2,2'-bpy)$_2$(4-ATP)$_2$.2PF$_6$ (I); (B) Ru(1,10-phen)$_2$(4-ATP)$_2$.2PF$_6$ (II)



A) UV λ_{max} (CH_3CN, ε mol^{-1} cm^{-1}): 252 nm (47909), 284 nm (60436), 418 nm (10552)
B) UV λ_{max} (CH_3CN, ε mol^{-1} cm^{-1}): 221 nm (79468), 263 nm (81584), 466 nm (10174)

Fig. S5 UV-vis spectra of, A)10^{-5} M Ru(1,10-phen)$_2$(dafo).2PF$_6$ (IV); (B) Ru(1,10-phen)$_2$(dah).2PF$_6$ (III) in acetonitrile.



A) UV λ_{max} (CH_3CN, ε mol^{-1} cm^{-1}): 223 (61774), 262 (63637), 436 (12687)
B) UV λ_{max} (CH_3CN, ε mol^{-1} cm^{-1}): 222 (72097), 261 (81642), 445 (16165)

Fig. S6 FT-IR spectral bands of , A) Ru(1,10-phen)$_2$(dafo)$_2$.2PF_6 (IV) complex ; B) Ru(1,10-phen)$_2$(dah).2PF_6 (III) complex

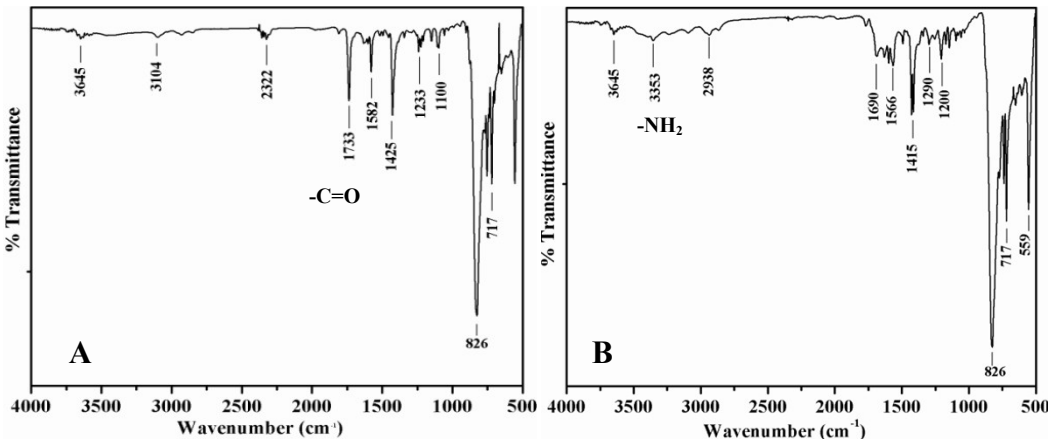


Fig. S7 Fluorescence emission profile of 10^{-5} M Ru(1,10-phen)$_2$(dah)·2PF_6 (III) in acetonitrile ($\lambda_{exc.}$ = 445 nm, λ_{em} = 600).

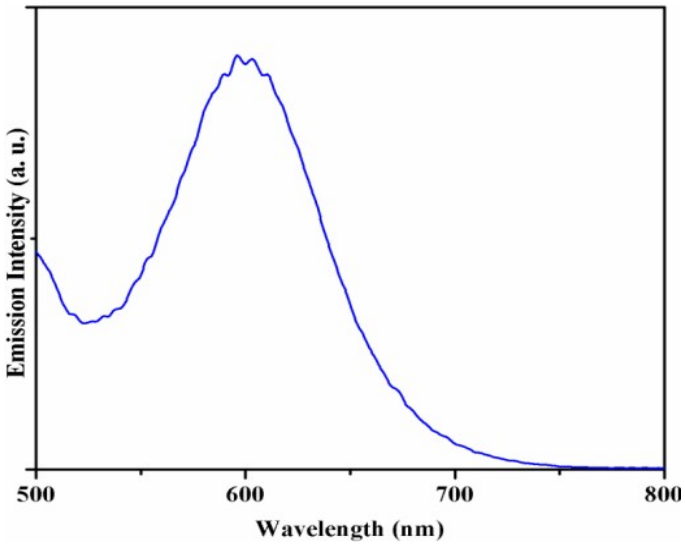
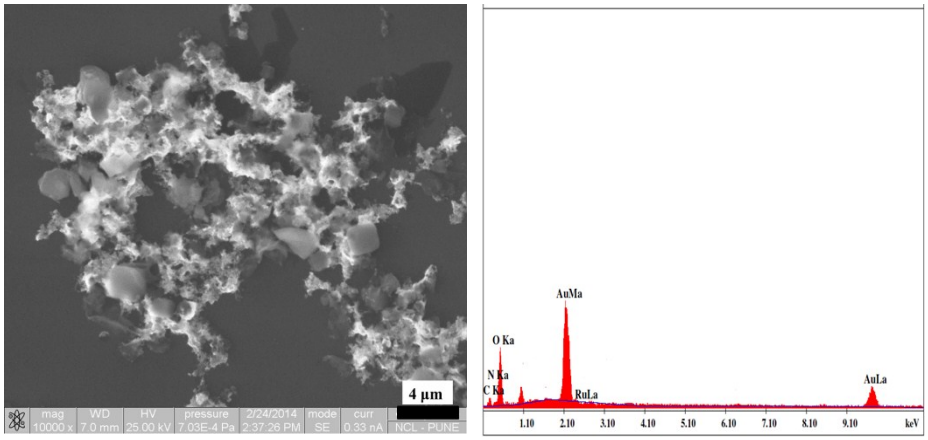


Fig. S8 SEM image and EDS analysis of functionalized Au NC cubes with random aggregates



Single crystal X ray crystallographic information: Single crystal X-ray diffraction data were collected at room temperature using a X-caliber-S OXFORD diffractometer Kappa CCD (at Delhi University). The apparatus was equipped with a graphite monochromator centered on the path of MoKα (λ = 0.71073 Å) with increasing ω (width 0.5 deg frame^{-1}). The single crystal was mounted on a fiber top with glue. The program Denzo-scalepack was used to integrate the data after an absorption correction with SADABS. The structure was solved by direct methods and refined by least squares on F^2 in SHELX97 and SHELX2013. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command.

Crystal structure of Ru(1,10-phen)$_2$(IPBA)(VI): This compound crystallizes in monoclinic crystal system under C2/c space group with a molecular formula of Ru(1,10-phen)$_2$(IPBA)·2 MeOH·6EtOH. The hexacoordinated Ru1 center is bonded with six N atoms, four of which are from 1,10-phen (N1 and N2) and rest two N atoms belong to IPBA ligand. The IPBA ligand lost two electrons, one from imidazole type amine (-NH) and other from the terminal carboxylate group (-COOH), therefore neutralizes the charge of the Ru(II) and forms neutral species Ru(1,10-phen)$_2$(IPBA). The Ru-N distances are 2.061(4) (Ru1-N1), 2.066(4) (Ru1-N2) and 2.051(4) (Ru1-N3) Å. There is total six ethanol molecule was found for each Ru(II) unit occupying the void spaces of the crystals. The electron density of the rest of the void

space are tried to assign with suitable and reasonable molecules and best assigned as two methanol molecule which are very close to each other. For these methanol molecules hydrogen atoms are not assigned on the oxygen, but those hydrogen are taken into account to calculate the molecular formula of the compound.

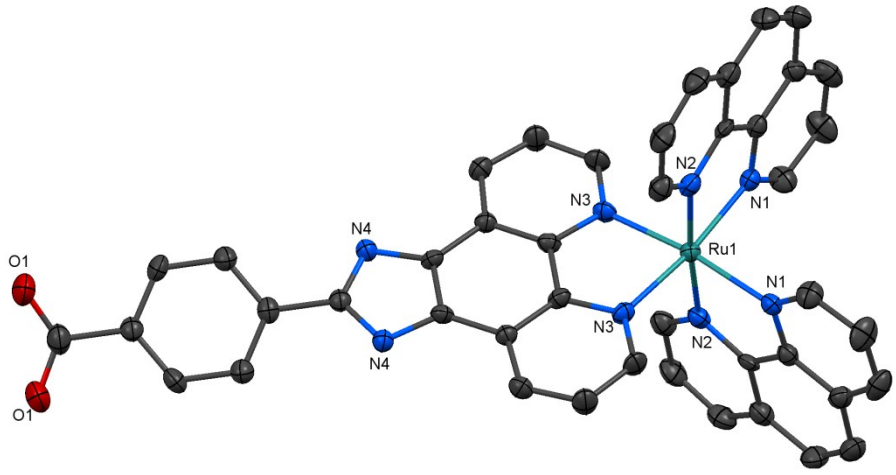


Fig. S9 ORTEP diagram of Ru(1,10-phen)$_2$(IPBA) molecule with thermal ellipsoids drawn 50% probability; green, blue, red and black sphere represents the Ru, N, O and C atoms. Solvent molecules and H-atoms are omitted for clarity.

Table S1. Single crystal parameters for Ru(1,10-phen)$_2$(IPBA)	
Formula	$C_{58}H_{70}N_8O_{10}Ru$
FW (g·mol^{-1})	1140.29
Crystal colour	orange
Crystal system, Space group	Monoclinic, C2/c
T (K)	293(2)
a (Å), b (Å), c (Å)	11.453(4), 25.177(5), 19.727(3)
β(°),	117.337(13)
V (Å^3), Z	5571(2), 4
Total refls.	4916
Unique refls. (I> 2σ(I))	3849
R_{int}	0.1006
R_1 (I> 2σ(I))	0.0722
wR_2 (all data)	0.1483
Goodness-of-fit	1.091
$^aR_1 = \Sigma\|\|F_o\| - \|F_C\|\|/\Sigma\|F_o\|$, and $^bwR_2 = [\Sigma w(F_o^2 - F_C^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ and $P = (F_o^2 + 2F_C^2)/3$	

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