

SUPPORTING INFORMATION

EBT anchored SiO₂ 3-D microarray: A simultaneous entrapper of two different metal centers at High and Low oxidation states using its respective highest occupied and lowest unoccupied molecular orbital

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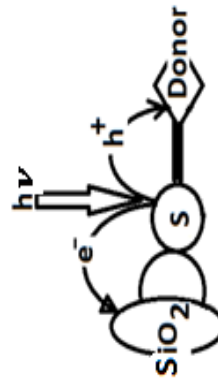
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Schemes:



Scheme S1



Scheme S2

File SI:

The specific surface area was calculated by the Brunauer-Emmett-Teller (BET) method using the adsorption branch.

BET (Specific Surface Area) Result: (t-Plot external surface area: 339.8254 m² g⁻¹; Single point surface area at P / P₀ of 0.300006229: 317.8206 m² g⁻¹; BJH adsorption cumulative surface area of pores between 17.0 A - 3000.0 A diameter: 324.381 m² g⁻¹ ; BJH desorption cumulative surface area of pores between 17.0 A - 3000.0 A diameter: 364.511 m² g⁻¹ and pore volumes (single point adsorption total pore volume of pores less than 1014.164 A diameter at P/P₀ of 0.980530216: 0.388974 cm³ g⁻¹; t-Plot micro pore volume: -0.007751 cm³ g⁻¹; BJH adsorption cumulative volume of pores between 17.0 A - 3000.0 A diameter: 0.374689 cm³ g⁻¹; BJH desorption cumulative volume of pores between 17.0 A - 3000.0 A diameter: 0.418756 cm³ g⁻¹) of the dry exchanger were obtained by BET analysis (Fig. 3c) and emphasizes the analytical application of the synthesized material. It also gives the pore sizes: 47.0107 A and 46.204 A respectively for the adsorption average pore width (4V/A by BET) and BJH adsorption average pore diameter (4V/A)).

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 Sample: EBT-D.O.S.Bag
 Operator: BOHTASHAWIK SINGH
 Submitter: DMSRDE HARG KANPUR P-60
 File: C:\02020\DDAT-1000-340\SMP

 Started: 7/10/2013 3:45:57PM
 Completed: 7/10/2013 7:49:01PM
 Report Time: 7/10/2013 1:54:17PM
 Sample Mass: 0.0710 g
 Cool Flow Space: 82.1653 cm³
 Low Pressure Dose: None
 Analysis Adsorptive: N2
 Analysis Bath Temp.: -156.850 °C
 Thermal Correction: No
 Warm Flow Space: 25.4410 cm³ Measured
 Equilibration Interval: 5 s
 Automatic Degas: Yes

Single point surface area at P/Po = 0.300006229: 317.8206 m²/g

BET Surface Area: 330.9668 m²/g

t-Plot External Surface Area: 339.8254 m²/g

BJH Adsorption cumulative surface area of pores between 17.000 Å and 3000.000 Å diameter: 324.391 m²/g

BJH Desorption cumulative surface area of pores between 17.000 Å and 3000.000 Å diameter: 364.5110 m²/g

Single point adsorption total pore volume of pores less than 1014.164 Å diameter at P/Po = 0.980530216: 0.388974 cm³/g

t-Plot micropore volume: 0.007751 cm³/g

BJH Adsorption cumulative volume of pores between 17.000 Å and 3000.000 Å diameter: 0.374689 cm³/g

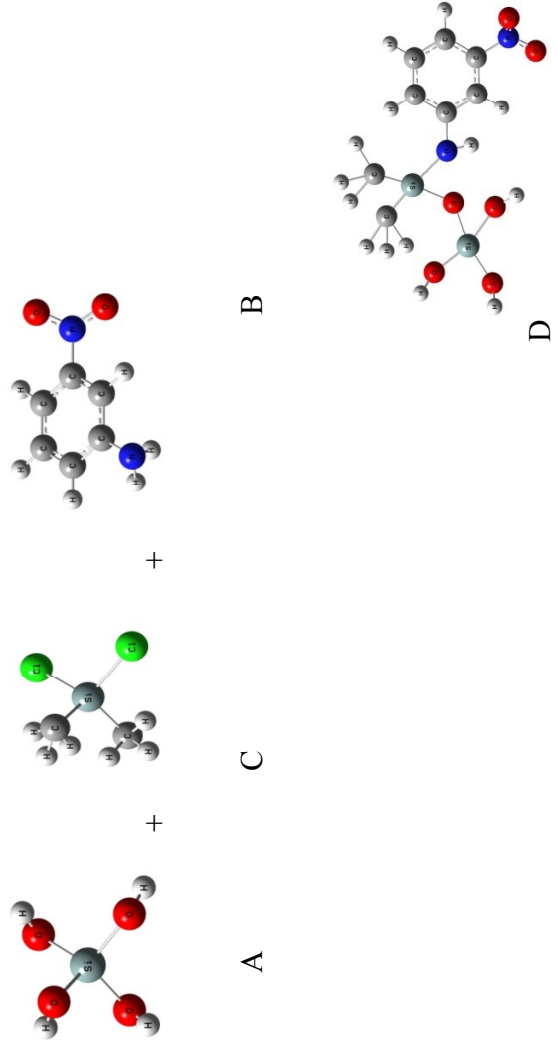
BJH Desorption cumulative volume of pores between 17.000 Å and 3000.000 Å diameter: 0.418756 cm³/g

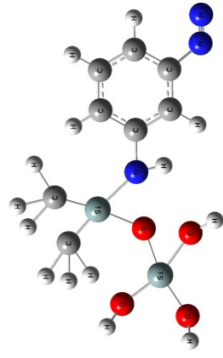
Pore Size

Adsorption average pore width (4V/A by BET): 47.0107 Å

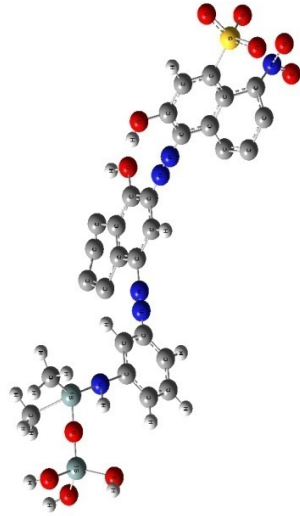
BJH Adsorption average pore diameter (4V/A): 46.204 Å

Scheme S3: Synthesis of the extractor: Chemical structure of Resin (FSG-EBT)





E (diazo-compound)



F (Resin: Diazo-EBT complex)

Scheme-S3 (synthesis of the resin)

Table S1: Selected experimental FT-IR and RAMAN bands of extractor (FSG-EBT) and B3LYP/6-STO-3G (d) calculated vibration modes with considerable Raman intensity.

RAMAN (Exp.) (cm⁻¹)	B3LYP (DFT) (cm⁻¹)	RAMAN / FTIR [50,51]	Band Assignment
FT-IR(Exp.) (cm⁻¹)	(Reported) (cm⁻¹)		
(1065, 1088) ^{a+} (1203) ^{b-}	(781, 1070) ^{a+} (1230) ^{b-}	(1075) ^{a+} (1201,1232) ^{b-}	Si-O-Si linkage ^[10]
(420,710,820) ^c	(450,705,840) ^c	(414,470,764,810) ^c	
(900-1203) ^{b+} (1100) ^{b-}	(850-1100) ^{b+} (1120) ^{b-}	(950-1200) ^{b+} (1080-1100) ^{b-}	Si-O ^[11a]
(2192) ^{a+} (2270) ^{b-}	(2000) ^{a+} (2150) ^{b-}	(2187) ^{a+} (2170) ^{b-}	Si-H ^[11b]
(1518, 1595) ^{a+} (1320) ^{b-}	(1500,1600) ^{a-} (1570) ^{b-}	(1505,1594) ^{a+} (1614) ^{a-}	-NO ₂
(1422, 1559) ^{b+}	(1450) ^{b+}	(1576) ^{b-} (1565, 1617) ^{b+}	
(1136) ^{a+} (1107,1559) ^{b+}	(1130) ^{a+} (1100,1550) ^{b-}	(1130) ^{a+} (1144,1540) ^{b+}	-S=O & -OH in -SO ₃ H (Silanol group)
(1120) ^{b-}	(1125) ^{b+}	(1145) ^{b-}	
(1281-1372) ^{a+} (1516-1570) ^{a-} (1559) ^{b-} (1320) ^{b+}	(1281-1372) ^{a+} (1500-1580) ^{a-} (1559) ^{b-} (1350) ^{b+}	(1293-1374) ^{a+} (1505-1594) ^{a-} (1501-1617) ^{b-} (1397) ^{b+}	-C-C-stretching of pyridine ring
(1518) ^{a+} (951,2031) ^{b-}	(1500) ^{a+} (800,2010) ^{b+}	(1505-1558) ^{a+}	-N=N-stretching ^[12] , amidst (i) EBT,EBT- diazotized
(1320) ^c	(1350) ^c	(884,2089,2123) ^{b-} (1335) ^c	FSG
(1450-1480) ^{a+} (1200) ^{b-}	(1400, 1435) ^{a+} (1250) ^{b-}	(1447-1470) ^{a+} (1274) ^{b-}	φ C-H stretching of pyridine ring.

(1136) ^{a+} (1050,1107) ^{b-}	(1160) ^{a+} (1050;1120) ^{b-}	(1144) ^{a+} (1049,1145) ^{b-} (803) ^c	O-H in SO ₃ H
(807) ^c	(830) ^c		
(3300) ^{a+} (3525) ^{b--}	(3400) ^{a+} (3540.51) ^{b--}	(3350) ^{a+} (3100-3500) ^{b-}	N-H in (Si-N(H)-C(ϕ -ring))
(1120) ^c	(1170) ^c	(1175) ^c	
(1137-1559) ^{a+} (1050-1559) ^c	(1110-1570) ^{a+} (1049-1650) ^c	(1144-1558) ^{a+} (1049-1617) ^c	Phenolic-OH of naphthol
((1137-1559) ^{a+}	(1100-1570) ^{a+}	(1144-1558) ^{a+} (803, 1049-	O-H in Si(OH) ₃
(816,1150-1559) ^{b-}	(840,1100-1595) ^{b-}	1617) ^{b-}	
(1050,1233,1291,1336) ^{a+}	(1054,1245,1360) ^{a+}	(1047, 1240, 1293, 1335) ^{a+}	C-N linkage ^[13]
(2350) ^{b-}	(2200) ^{b-}	(2200) ^{b-}	
(858-1203) ^{b-}	(850-1180) ^{b-}	(862-1170) ^{b-}	Si-N stretching ^[14]
(978,1012-1614) ^{a+}	(1017-1620) ^{a+} (3600) ^{b+}	(973,1007-1614) ^{a+} (3655-	C-H of aliphatic CH ₃ attached to Si ^[15]
(3697) ^{b-} (951-1632) ^c	(1050-1559) ^c	3699) ^{b-} (1047-1594) ^c	

a = Raman; b = FT-IR; c = bending; -ve = sym. Stretching; +ve = assym. Stretching; ϕ = aromatic

Figure S1: Experimental Raman spectra (Experimental Raman Spectra (upper curve corresponds to the Th-loaded exchanger

while lower curve corresponds to the unloaded exchanger))

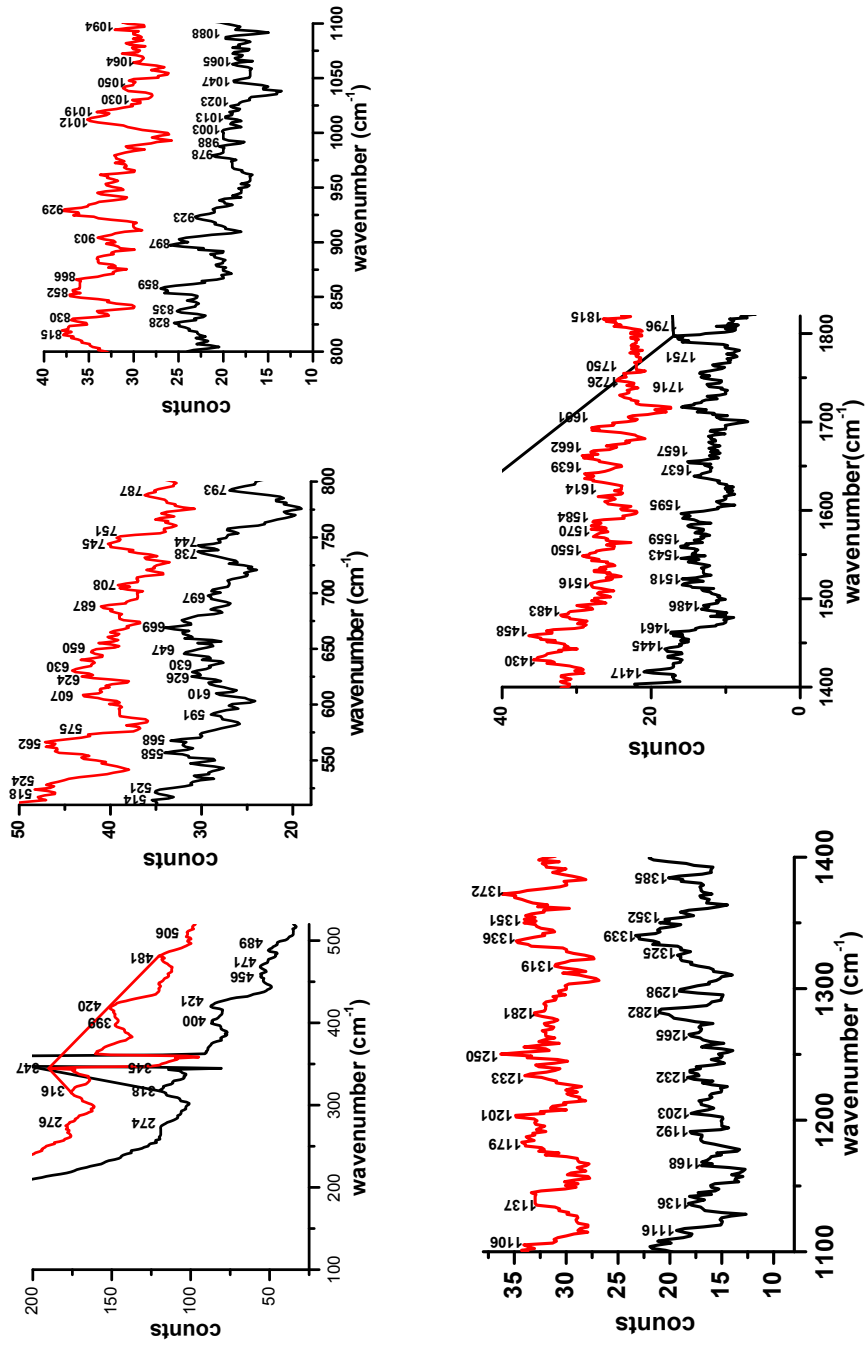
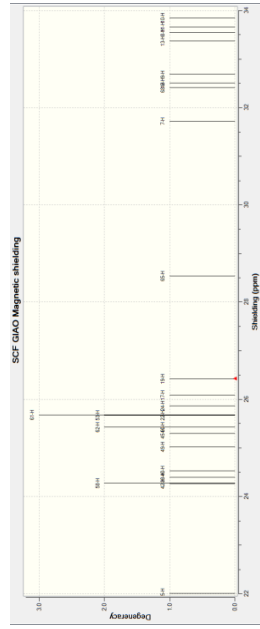
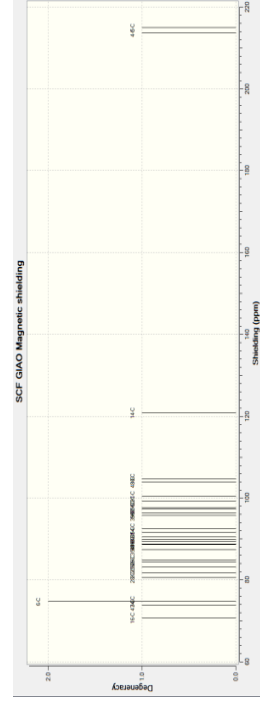


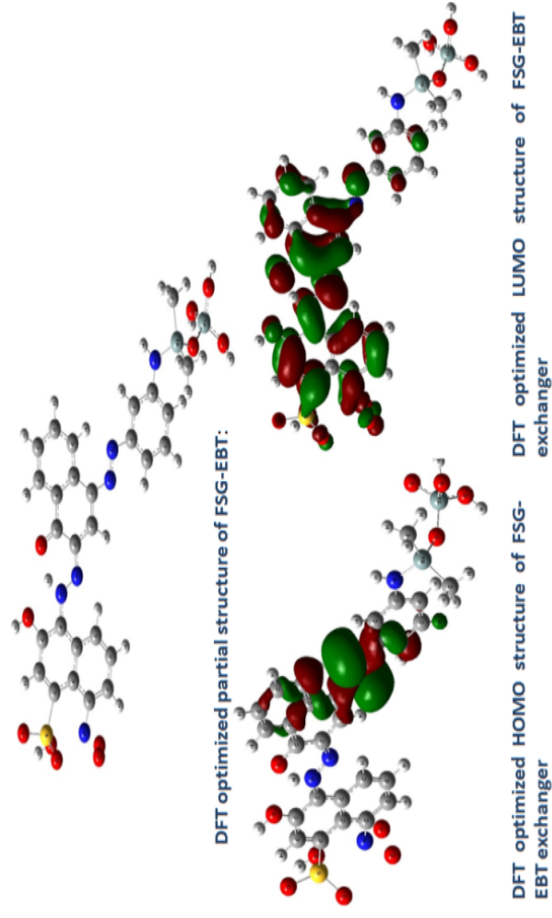
Figure S2: DFT calculated NMR spectra of ^1H (a) and ^{13}C NMR (b) of a model compound (c) comprising one tetrahedral edge of FSG-EBT used in DFT calculation for NMR spectra.



(a)



(b)



(c)

[Considering the symmetry properties of the molecule only one tetrahedral edge of FSG-EBT was taken as a model compound (Figure S2 c) to have the NMR spectra from DFT calculation. In the DFT NMR spectra (Figure S2 (a-b)) there are six pair of aromatic carbons of similar δ (ppm) values in its ^{13}C spectrum [84.8986 and 84.4461 for (C52 & C26); 74.7593 and 74.7813 for (C34 & C6); 88.6252 and 88.7531 for (C59 & C41); 97.7202 for (C57 & C15); 89.3824 and 89.8880 for (C46 & C18); 95.7599 and 96.4242 for (C39 & C56)] suggesting the shortage of 6 aromatic carbons in experimental spectra (^{13}C NMR) and clearly confirms the molecular structure

13C OF BM/FSG1

118.8
122.20
129.81
131.26
132.76

122.04



 13C NMR Spectrum
 Sample: BM/FSG1
 Date: 01/15/2004
 Time: 14:30
 Solvent: CDCl3
 Concentration: 10 mg/ml
 Temperature: 25°C
 Acquisition: 128 K, 128 F, 128 S, 128 T, 128 U, 128 V, 128 W, 128 X, 128 Y, 128 Z
 Processing: 128 A, 128 B, 128 C, 128 D, 128 E, 128 F, 128 G, 128 H, 128 I, 128 J, 128 K, 128 L, 128 M, 128 N, 128 O, 128 P, 128 Q, 128 R, 128 S, 128 T, 128 U, 128 V, 128 W, 128 X, 128 Y, 128 Z
 Reference: 128 AA, 128 AB, 128 AC, 128 AD, 128 AE, 128 AF, 128 AG, 128 AH, 128 AI, 128 AJ, 128 AK, 128 AL, 128 AM, 128 AN, 128 AO, 128 AP, 128 AQ, 128 AR, 128 AS, 128 AT, 128 AU, 128 AV, 128 AW, 128 AX, 128 AY, 128 AZ
 Integration: 128 BA, 128 BB, 128 BC, 128 BD, 128 BE, 128 BF, 128 BG, 128 BH, 128 BI, 128 BJ, 128 BK, 128 BL, 128 BM, 128 BN, 128 BO, 128 BP, 128 BQ, 128 BR, 128 BS, 128 BT, 128 BU, 128 BV, 128 BW, 128 BX, 128 BY, 128 BZ
 Scale: 128 CA, 128 CB, 128 CC, 128 CD, 128 CE, 128 CF, 128 CG, 128 CH, 128 CI, 128 CJ, 128 CK, 128 CL, 128 CM, 128 CN, 128 CO, 128 CP, 128 CQ, 128 CR, 128 CS, 128 CT, 128 CU, 128 CV, 128 CW, 128 CX, 128 CY, 128 CZ
 Name: 128 DA, 128 DB, 128 DC, 128 DD, 128 DE, 128 DF, 128 DG, 128 DH, 128 DI, 128 DJ, 128 DK, 128 DL, 128 DM, 128 DN, 128 DO, 128 DP, 128 DQ, 128 DR, 128 DS, 128 DT, 128 DU, 128 DV, 128 DW, 128 DX, 128 DY, 128 DZ
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 Operator: 128 FA, 128 FB, 128 FC, 128 FD, 128 FE, 128 FF, 128 FG, 128 FH, 128 FI, 128 FJ, 128 FK, 128 FL, 128 FM, 128 FN, 128 FO, 128 FP, 128 FQ, 128 FR, 128 FS, 128 FT, 128 FU, 128 FV, 128 FW, 128 FX, 128 FY, 128 FZ
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 Disk: 128 LA, 128 LB, 128 LC, 128 LD, 128 LE, 128 LF, 128 LG, 128 LH, 128 LI, 128 LJ, 128 LK, 128 LL, 128 LM, 128 LN, 128 LO, 128 LP, 128 LQ, 128 LR, 128 LS, 128 LT, 128 LU, 128 LV, 128 LW, 128 LX, 128 LY, 128 LZ
 Drive: 128 MA, 128 MB, 128 MC, 128 MD, 128 ME, 128 MF, 128 MG, 128 MH, 128 MI, 128 MJ, 128 MK, 128 ML, 128 MM, 128 MN, 128 MO, 128 MP, 128 MQ, 128 MR, 128 MS, 128 MT, 128 MU, 128 MV, 128 MW, 128 MX, 128 MY, 128 MZ
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 File Path: 128 PA, 128 PB, 128 PC, 128 PD, 128 PE, 128 PF, 128 PG, 128 PH, 128 PI, 128 PJ, 128 PK, 128 PL, 128 PM, 128 PN, 128 PO, 128 PP, 128 PQ, 128 PR, 128 PS, 128 PT, 128 PU, 128 PV, 128 PW, 128 PX, 128 PY, 128 PZ
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(b)

Figure S4: TD-DFT UV-Vis spectra of FSG-EBT

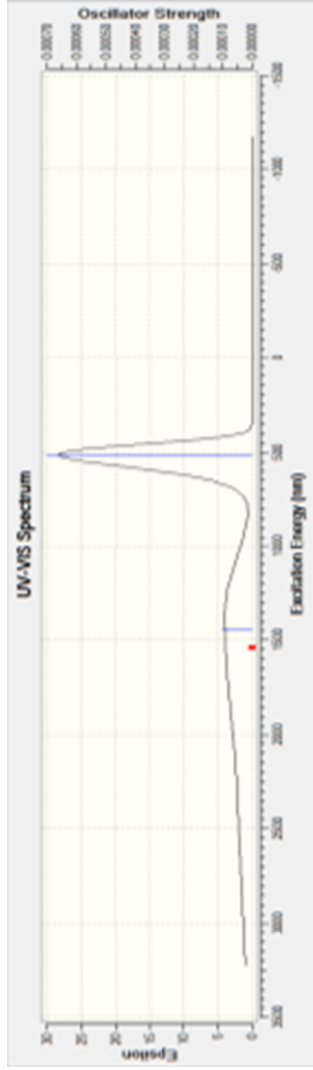
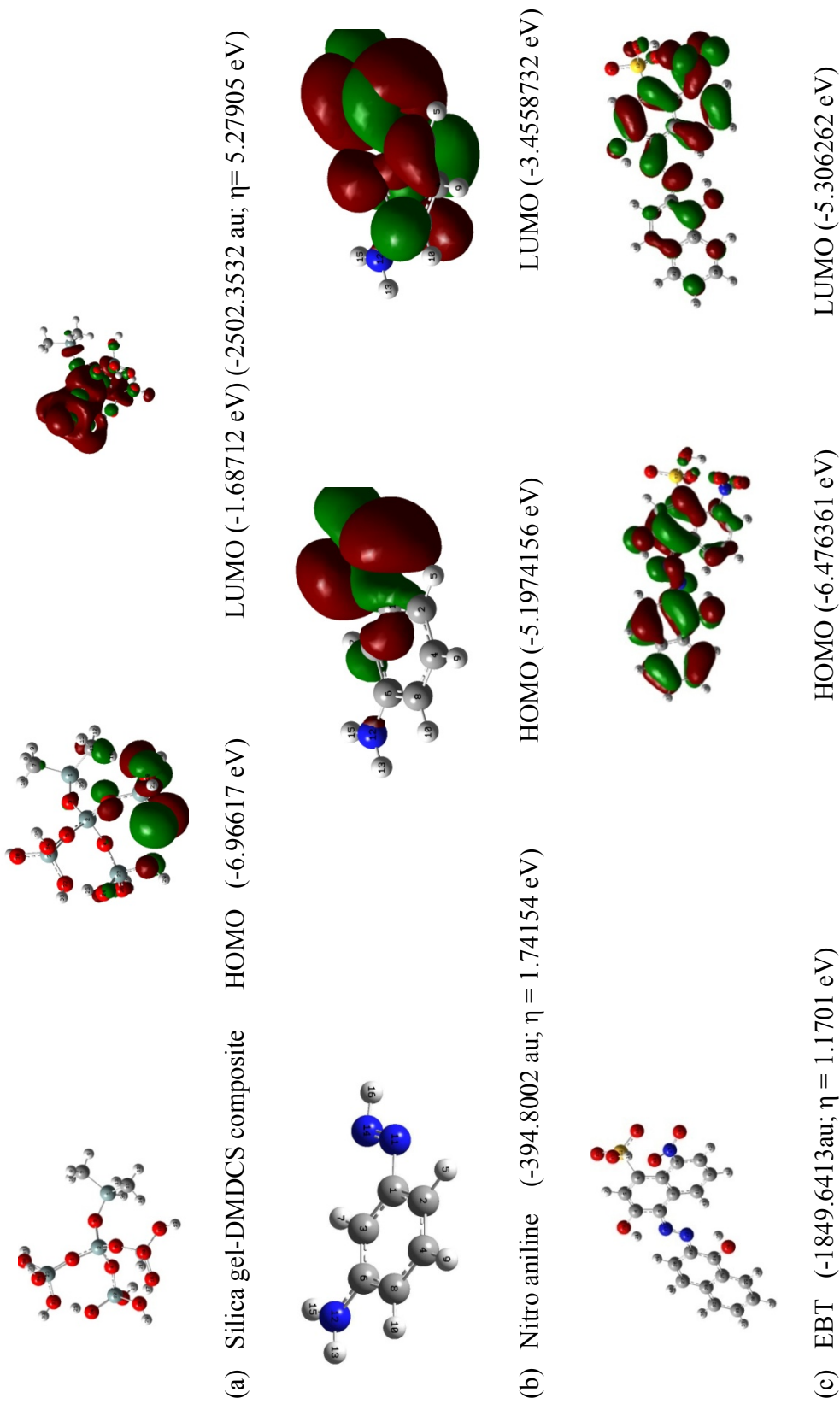
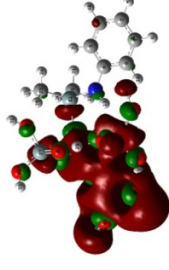
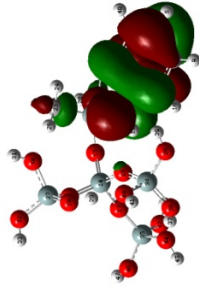
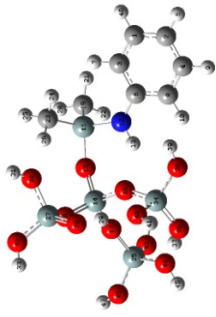


Figure S5: (a-i) DFT optimized structures of the relevant building units of the resin

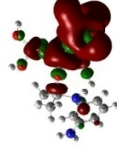
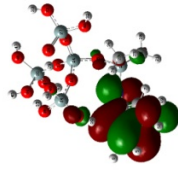
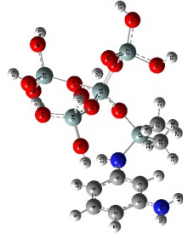




(d) SG-DMDCS-aniline (-2787.15324 au; $\eta = 3.183757$ eV)

HOMO (-5.0885692 eV)

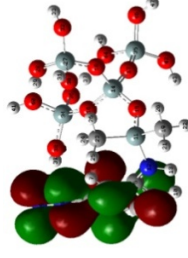
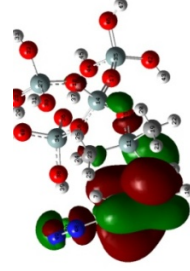
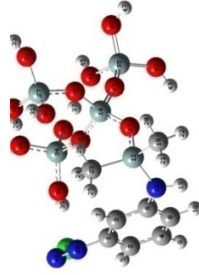
LUMO (-1.9048120 eV)



(e) Silica-DMDCS-m-aminoaniline (-2842.2366 au; $\eta = 3.5919312$ eV)

HOMO (-5.2246272 eV)

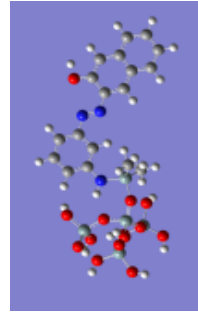
LUMO(-1.632696 eV)



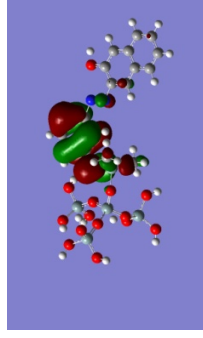
(f) Silica-DMDCS- m-aminoaniline-chloride (3354.4602 au; $\eta = 1.98643$ eV)

HOMO (-6.1770332 eV);

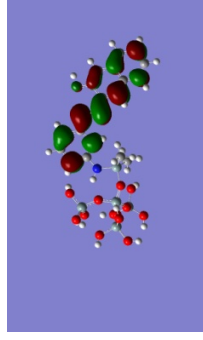
LUMO (-4.1906 eV)



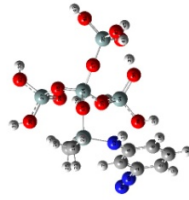
(g) Silica-m-diazonaph-aniline ($\eta = 1.7252$ eV)



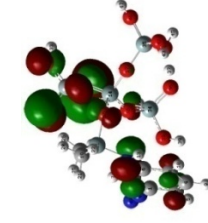
HOMO (-5.2319 eV)



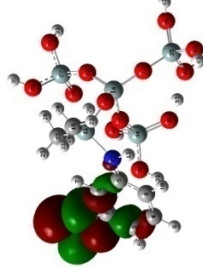
LUMO (3.5068 eV)



(h): Chloride salt of (g) (-3936.4161 a.u.; $\eta = 2.5842$)



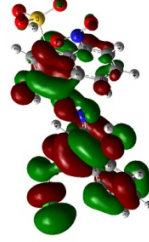
HOMO (-9.3063672 eV)



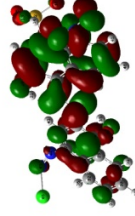
LUMO (-8.571654 eV)



(i) EBT diazo
(-2416.92 au; 11.06 Debye)



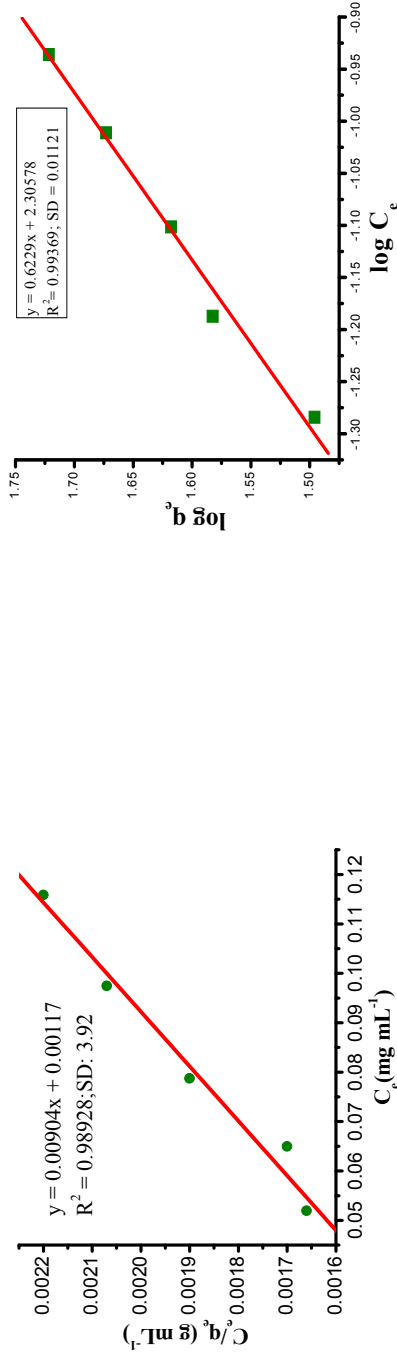
HOMO (-6.8573 eV)



LUMO (-5.6872 eV)

[In all the building moieties viz. SG, linker (m-diazoaniline) and azo-dye (EBT) HOMO-LUMO are not well separated (Figure S5 (a-d)). However, in course of their attachment, HOMO resides at the linker site at every occasion whereas LUMO gradually shifts its position from silanized silica part to the dye component (Figure S5 (d-i)) and finally in the synthesized resin HOMO-LUMO get well separated (Figure 6a-d). Thus, both charge and hole are transferred through a 'quasi-equilibrium' [60] as per Scheme-s1, and suggests the longer life time of the ejected electron placed at the SiO₂ moiety. The expected charge transfer from the different components of the material produce spectral lines at the UV-Vis range (3.5919(348.0); 3.1837(392.6); 1.9864(629.3); 1.4967(835.2 nm) and 1.0701 eV (1168.1 nm)) corresponding to their HOMO-LUMO band gap (Figure S4). The experimental spectral positions (274, 366.4, 450, 578, 880.5, 950.3 and 1094.5 nm) (Figure 7a-b) are nearly compatible and support the transfer of hole by *hopping mechanism*. The privileges, thus highlighted, along with the intra-molecular charge/hole transfer can be exploited for its utility as a LED source.]

Figure S6: Sorption isotherms:



(a)

(b)

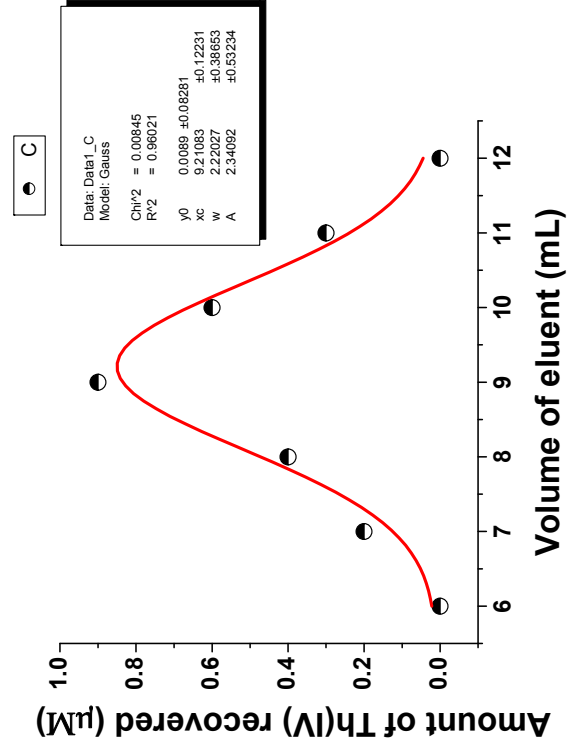
(a) Plot of C_e (mg mL^{-1}) vs. $\frac{C_e}{q_e}$ (g mL^{-1}) for Langmuir isotherm (b) plot of $\log C_e$ ($\mu\text{mol mL}^{-1}$) vs. $\log q_e$ ($\mu\text{mol g}^{-1}$) for

Freundlich isotherm ($\log q_e = \log K_F + \frac{1}{n} \log C_e$; $K_F = 1.25 \times 10^2$ and $n = 1.61$)

Table S2: Langmuir and Freundlich parameters

Langmuir parameters ; $R^2 = 0.9893$				Freundlich parameters; $R^2 = 0.9936$					
C_e	q_e	Q_0 (mg g^{-1})	b (L mg^{-1})	$q_{e(t)}$	RMSE	$\frac{1}{n}$	k_F	$q_{e(t)}$	RMSE
0.052	31.3253	110.6195	7.7265	31.7057	0.8857	0.623	2.02×10^2	32.0614	0.9636
0.0650	38.2853	476.7 ($\mu\text{M g}^{-1}$)		36.9822				36.8424	
0.0788	41.4737			41.8625				41.6635	
0.0975	47.1015			47.5285				47.4279	
0.1159	52.6818			52.2605				52.8204	

Figure S7: Elution profile of Th (IV)



[0.5mol L⁻¹ HClO₄; total volume: 5 mL; Peak height: 0.84124]

Plate number, $N = 4 \times \left[\frac{y^2}{x^2} \right] = 296$; Where, $x = \frac{1}{2} \times w_{0.6065x/h}$; $w_{0.6065x/h}$ = width at a 0.6065 times of peak height; y = distance for peak

elution.