Supplementary Information

Insights into the Multifunctional Applications of Strategical Co doped MoS₂ Nanoflakes

R. Rahman¹, S. Chowdhury¹, D. Samanta², A. Pathak² and T. K. Nath^{*1}

¹Department of Physics, Indian Institute of Technology Kharagpur, West Bengal 721302, India ²Department of Chemistry, Indian Institute of Technology Kharagpur, West Bengal 721302, India

S1 XRD data analysis



Fig. S1 Magnified image of XRD plot indicating evolution of 1T phase in 2H phase MoS_2 with increase in Co doping.

S2. VSM data



Fig. S2 M vs H hysteresis loop of (a) undoped MoS₂, (b) 2% Co, (c) 6% Co at 10K, 100 K and 300 K within applied magnetic field range of -2T to 2 T. (d), (e), (f) represent $1/\chi$ vs T plot corresponding to undoped, 2% Co doped MoS₂ (paramagnetic nature) and 6% Co doped MoS₂ (ferromagnetic nature); inset of (f) shows minima of dm/dT plot indicating T_c of 6% Co doped MoS₂ NFs at 131 K.

S3 Theoretical result



Fig. S3 Total density of states (TDOS) of (a) undoped MoS_2 supercell; (b) the supercell with 2% Co dopant; (c) the supercell with 6% Co and (d) the supercell with 8% Co dopant atom (the vertical dashed line indicates the Fermi level).

S4 Electrochemical analysis



Fig. S4 Left panel shows the CV curves of (a) undoped, (c) 2% Co (e) 4% Co doped MoS₂ at different scan rates; Right panel shows the GCD profile of (b) undoped MoS₂ and (d) 2% Co doped (f) 4% Co doped MoS₂ at different current densities.

Scan rate	$C_{sp}(MoS_2)$	C _{sp} (2% Co)	C _{sp} (4% Co)	C _{sp} (8% Co)
(mV/s)	(F/g)	(F/g)	(F/g)	(F/g)
100	41.4	71.4	79.3	102.2
80	58.1	82.3	85.2	114.02
60	66.8	88.4	89.44	128.7
40	72.5	98.3	102.08	148.8
20	85.9	111.2	127.5	180.5
10	98.1	123.8	162.8	217.9

Table S1 Specific capacitance (C_{sp}) values at different scan rates for undoped, 2% Co, 4% Coand 8% Co doped MoS2 (From CV plots)

 $\label{eq:Table S2} \begin{array}{l} \mbox{Table S2} \ \mbox{Time of discharge current values and specific capacitance at different current densities for undoped, 2% Co, 4% Co and 8% Co-doped MoS_2 \end{array}$

Undoped		2% Co		4% Co			8% Co				
Current	Δt	C _{sp}									
density	(sec)	(F/g)									
(A/g)			(A/g)			(A/g)			(A/g)		
0.7	51	59.5	0.7	85	99.1	1.5	64	162.5	1.5	187	201.4
1.5	12	18	1	53	88.3	3	23	115	3	82	173.6
2	6	15	2	22	73.3	4	11	66.7	4	48	137.1
3	3	11.3	5	5	41.6	5	8	58.3	6	29	124.3
						6	5	50	14	7	70