

Supporting Information

MWCNT Intercalated Natural Hematite-based Activable Nanocomposite for Piezoelectric Energy Generation and ROS-Mediated Carcinogenic Dye Degradation

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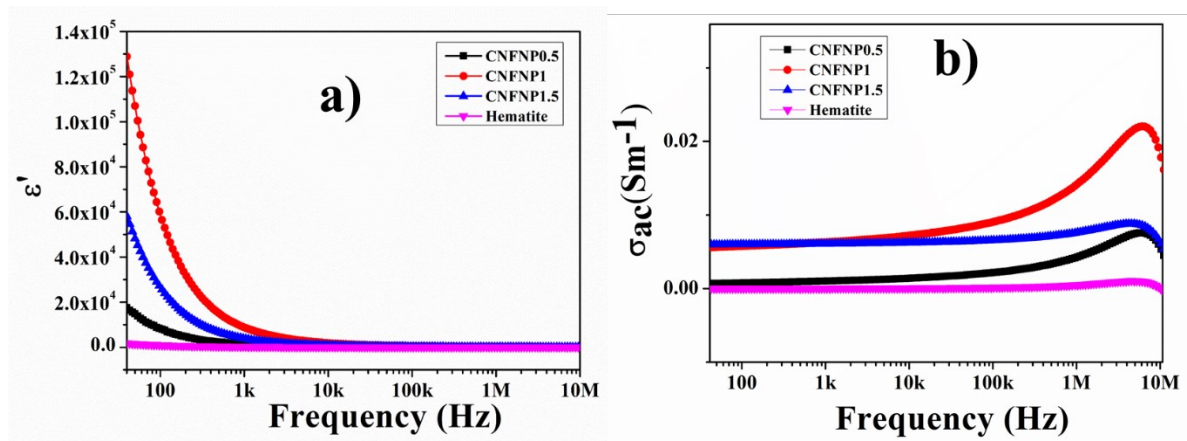
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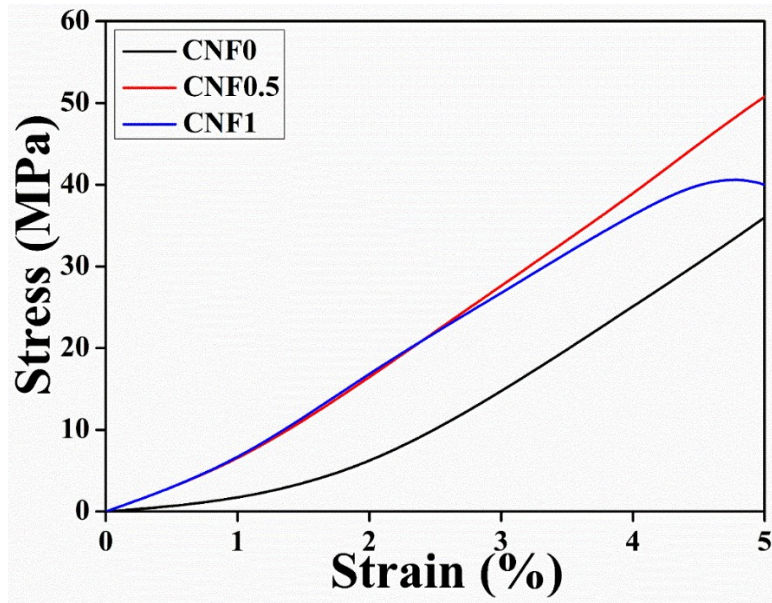
Figure S1: a) Dielectric constant and b) AC conductivities of MWCNT incorporated hematite nano-rock



S2: Electrical properties of MWCNT-incorporated hematite nano-rock

To obtain the maximum efficient nanocomposite, 0.5, 1, and 1.5 % wt/wt MWCNT have been incorporated into hematite nano-rock by the condensation technique procedure discussed in the main manuscript in the material synthesis portion and named as CNFNP0.5, CNFNP1.0, and CNFNP1.5 respectively. Figure S1 depicted that the incorporation of MWCNT enhances the electrical polarization properties with MWCNT percentage and found maximum in 1% MWCNT doped nanocomposite. Thus, this sample has been incorporated into PVDF matrix for fabricating nanocomposite membranes.

Figure S3: Stress-strain graphs of CNT incorporated α -hematite



S4: Formulation of calculation of force

The velocity was determined using the conservation of energy formula,

$$mgh = \frac{1}{2} mv^2 \dots\dots\dots(1)$$

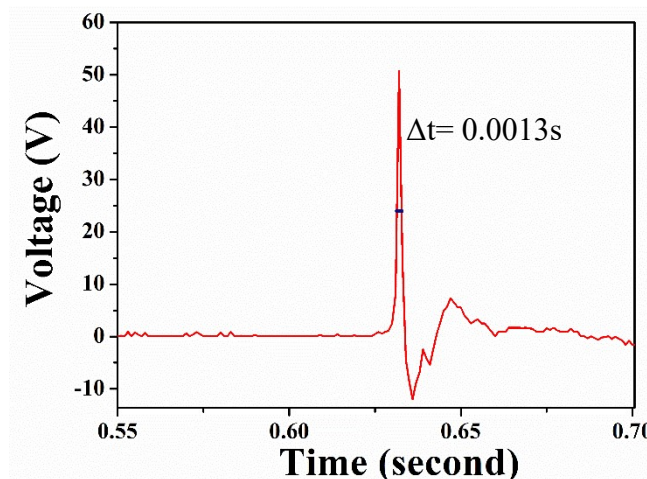
Where m, g, and h are the mass, the gravitational constant, and the height respectively from whence the mass imparted the membrane, and v is the velocity.

$$mv = (F-mg) \Delta t \dots\dots\dots(2)$$

$$F = m (v/\Delta t + g) \dots\dots\dots(3)$$

Initially, applying the m= 0.015 kg, h=0.1 m, and Δt is the impulsive time derived from the open circuit voltage graph (FWHM) and discovered Δt= 0.0013s

Figure S5: Impulsive time calculation



We estimated the force using Equation 3 and found it to be 16.3 N.

S6: DFT data of PCNF 0

CARTESIAN COORDINATES (ANGSTROEM)

C	-12.194185	-2.766798	1.713114
C	-11.791043	-1.365812	1.283341
H	-12.185368	-3.447424	0.856618
H	-13.203654	-2.734075	2.132842
H	-11.508243	-3.142586	2.477392
C	-10.395183	-1.299614	0.658407
C	-9.769698	0.090510	0.486821
H	-10.453995	-1.793140	-0.316888
H	-9.709575	-1.881654	1.282532
C	-8.492996	-0.005203	-0.360972
C	-7.666419	1.272072	-0.566265
H	-8.774240	-0.382691	-1.349858
H	-7.846564	-0.754926	0.107793
C	-6.310263	0.943254	-1.209644
C	-5.404311	2.121950	-1.580927
H	-6.480938	0.358806	-2.119989
H	-5.768021	0.305146	-0.505026
C	-3.987453	1.673594	-1.938933
C	-2.939295	2.775792	-2.135182
H	-4.045682	1.101587	-2.871069
H	-3.624487	0.992987	-1.159667
C	-2.494309	3.480981	-0.829551
C	-0.981718	3.666421	-0.628578
H	-2.877567	2.947428	0.045248
H	-2.936334	4.480960	-0.794567
C	-0.238278	2.368991	-0.298953
C	1.238262	2.465126	0.103423
H	-0.322977	1.725270	-1.175821
H	-0.763056	1.877311	0.526894
C	1.878691	1.067650	0.109853

C	3.299450	0.956501	0.675657
H	1.886141	0.703497	-0.922780
H	1.236769	0.398362	0.692208
C	3.879342	-0.449970	0.445954
C	5.311480	-0.685384	0.945210
H	3.850692	-0.656251	-0.629030
H	3.227466	-1.175656	0.943574
C	5.839906	-2.074470	0.554732
C	7.327946	-2.317187	0.787134
H	5.641083	-2.251506	-0.507508
H	5.282055	-2.823423	1.126193
F	-11.859298	-0.537039	2.374871
F	-12.710079	-0.902965	0.371044
F	-9.473864	0.593201	1.724362
F	-10.652651	0.953223	-0.097591
F	-7.448294	1.885253	0.635935
F	-8.358537	2.149107	-1.353757
F	-5.937610	2.795117	-2.652488
F	-5.355286	3.016722	-0.538455
F	-1.848931	2.118034	-2.738974
H	-3.288347	3.512306	-2.864797
F	-0.435987	4.263638	-1.732062
F	-0.836528	4.553002	0.412782
F	1.347989	3.019998	1.348311
F	1.912435	3.283251	-0.758860
F	3.285553	1.228509	2.016354
F	4.097823	1.890770	0.081965
F	5.336995	-0.564355	2.309255
F	6.138345	0.276046	0.437862
F	7.658210	-2.104642	2.092384
F	8.089889	-1.490353	0.014583
H	7.600756	-3.349327	0.533424

S7: DFT data of PCNF 0.5

CARTESIAN COORDINATES (ANGSTROEM)

C	-8.333444	1.455904	-0.365927
C	-7.820822	1.777806	1.036261
C	-6.301395	1.742656	1.168256
H	-8.263310	1.083027	1.758346
H	-8.143861	2.786611	1.313743
C	-5.670133	0.349465	1.203891
C	-4.141501	0.274280	1.092093
H	-6.102608	-0.270434	0.411817
H	-5.938660	-0.110653	2.160208
C	-3.566048	0.539442	-0.297499
C	-2.043754	0.485264	-0.458240
H	-3.866839	1.538916	-0.613686
H	-4.010703	-0.176601	-0.995742
C	-1.358450	-0.867552	-0.259655
C	0.167291	-0.893972	-0.425462
H	-1.795305	-1.584677	-0.961913
H	-1.572085	-1.226235	0.749453
C	0.721490	-0.531300	-1.803586
C	2.216422	-0.216969	-1.894379
H	0.216446	0.363064	-2.168430
H	0.484864	-1.347576	-2.493341
C	3.210014	-1.316485	-1.519589
C	4.640932	-0.812471	-1.282613
H	3.235729	-2.035862	-2.343757
H	2.864424	-1.844744	-0.627387
C	4.905967	-0.320661	0.135827
C	6.192639	0.480883	0.357584
H	4.927072	-1.200139	0.785823
H	4.085255	0.322522	0.461486
C	7.474856	-0.037582	-0.293825
C	8.728433	0.810111	-0.060766
H	7.321390	-0.072350	-1.374669
H	7.663846	-1.059525	0.047655
C	9.315232	0.824923	1.347093
C	10.388490	1.886672	1.590357
H	9.740665	-0.163037	1.551243

H 8.522058 1.008373 2.073305
 C 11.509306 1.967173 0.556438
 F -9.720763 1.489398 -0.354099
 H -8.022494 0.458613 -0.701352
 H -7.973616 2.195526 -1.087762
 F -5.963133 2.414302 2.311329
 F -5.764972 2.462120 0.108915
 F -3.801600 -1.019440 1.461513
 F -3.575822 1.101134 2.015514
 F -1.822575 0.900404 -1.765873
 F -1.470962 1.424856 0.345031
 F 0.550971 -2.196678 -0.128526
 F 0.737650 -0.110298 0.538274
 F 2.465840 0.908138 -1.144258
 F 2.441549 0.134626 -3.204422
 F 4.973511 0.148304 -2.202401
 F 5.497994 -1.870469 -1.526650
 F 5.975411 1.771365 -0.029636
 F 6.365021 0.509581 1.734732
 F 8.499968 2.091036 -0.487070
 F 9.697877 0.299931 -0.915526
 F 10.944436 1.623877 2.820046
 F 9.784100 3.110225 1.696058
 F 12.469637 2.856228 0.998013
 H 11.102423 2.316916 -0.394795
 H 11.967786 0.981441 0.420264

S8: Table of Piezoelectric coefficient measurement by specific capacitance and remnant polarizations

Sample code	Young modulus (MPa/mm)	Remnant polarization (P_r : $\mu\text{C}/\text{cm}^2$)	d_{33} ($C_p V/F$) (pC/N)	d_{33} ($-P_r/Y$) (pC/N)
CNF0	726	0.07	7.2	9.6
CNF0.5	124	0.15	127.6	121.0

CNF1	263	0.09	35.0	34.2
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Figure S9: a) Frequency, and b, c) force-dependent piezoelectric voltage generation by the device

