Electronic Supplementary Material (ESI) for RSC Advances.

Table S1 The geometrical parameters (bond lengths (R) is in Å), adsorption (E_{ad}) calculated at the B3LYP-D/6-31G* level

	$R_{C\text{-}Si}$	$R_{CS2\ldots nanotube}$	$R_{C\text{-}S}$	E_{ad}
Configuration 1	C1-Si2=1.812 C1-Si6=1.785	Si2…S18=3.446	C17-S19=1.561 C17-S18=1.561	-30.29
Configuration 2	C1-Si2=1.941 C1-Si6=1.901	C1…C17=1.486 Si2...S18=2.401	C17-S19=1.741 C17-S18=1.695	-604.201
Configuration 3	C1-Si2=1.787 C1-Si6=1.847	Si6…S18=2.260	C17-S19=1.575 C17-S18=1.666	57.117
Configuration 4	C1-Si2=1.814 Si2-C10=1.782	S18…C=3.376 S19…C13=3.952	C17-S19=1.553 C17-S18=1.598	5.468
Configuration 5	C1-Si2=1.973 C1-Si6=1.947	C1…C17=1.476 Si6…S19=2.289	C17-S19=1.729 C17-S18=1.710	-24.172
Configuration 6	C1-Si2=1.853 C3-Si2=1.998	Si2…C17=1.926 C3…S18=1.879	C17-S19=1.625 C17-S18=1.793	-458.44
Configuration 7	C1-Si2=1.814 C1-Si6=1.786	C1…S19= 4.657	C17-S19= 1.598 C17-S18= 1.553	5.463
Configuration 8	C1-Si2=1.810 Si2-C3=1.786	Si2…S17=3.601	C17-S19=1.565 C17-S18=1.560	9.603
Configuration 9	C1-Si2= 1.901 Si6-C1= 1.936	S19…C1=1.835	C17-S19= 1.659 C17-S18= 1.739	932.106
Configuration 10	C1-Si2= 1.804	S18…Si2= 3.025	C17-S19= 1.544 C17-S18= 1.573	329.207

Table S2 The geometrical parameters (bond lengths (R) is in Å), adsorption (E_{ad}) calculated at the CAM-B3LYP /6-31G* level

	$R_{C\text{-}Si}$	$R_{CS2\ldots nanotube}$	$R_{C\text{-}S}$	E_{ad}
Configuration 1	C4-Si5=1.834 C5-Si6=1.764	C5…S18=3.723	C17-S19=1.556 C17-S18=1.556	-25.39
Configuration 2	C5-Si4= 1.949 C5-Si6=1.886	C5…C17=1.484 Si4...S18=2.424	C17-S19=1.736 C17-S18= 1.672	-172.853
Configuration 3	C1-Si2=1.776 C1-Si6=1.843	Si6…S18=2.219	C17-S19=1.598 C17-S18=1.669	11.04
Configuration 4	C1-Si2=1.829 Si2-C10=1.766	S19…C10=4.070 C17…Si7=4.033	C17-S19=1.556 C17-S18=1.553	-2.662
Configuration 5	C1-Si2=1.980 C1-Si6=1.941	C1…C17=1.477 Si6…S19=2.238	C17-S19=1.731 C17-S18=1.677	-50.37
Configuration 6	C1-Si2=1.865 C3-Si2=1.980	Si2…C17=1.919 C3…S18=1.856	C17-S19=1.615 C17-S18=1.776	-29.75
Configuration 7	Si6-C11= 1.826 C11-Si20= 1.779	S19-Si20=2.677	C17-S19=1.578 C17-S18=1.532	-10.43
Configuration 8	C1-Si2= 1.831 Si2-C3=1.764	C3…S18= 4.105	C17-S19=1.560 C17-S18=1.551	-3.935
Configuration 9	C5-Si4=1.908 Si6-C5= 1.918	S19…C5=1.809	C17-S19=1.776 C17-S18=1.836	890.625
Configuration 10	C1-Si7= 1.785	S18…Si7=3.082	C17-S19= 1.517 C17-S18= 1.587	320.99

Table S3 energy of the highest occupied molecular orbital (E_{HOMO}) , energy of the lowest unoccupied molecular orbital (E_{LUMO}), the molecular orbital energy gap, Eg, Chemical hardness (η) and chemical potential (μ), Fermi level energy and work function (Φ) in terms of eV computed at B3LYP-D

	E_{HOMO}	E_{LUMO}	Eg	η	μ	E_{FL}	φ
Configure1	-4.24075	-3.8738	0.36690	0.183460	-4.05729	-4.05729	4.05729
Configure2	-4.16949	-3.81643	0.353056	0.176528	-3.99296	-3.99296	3.99296
Configure3	-4.2179	-3.85941	0.358496	0.179248	-4.03866	-4.03866	4.038656
Configure4	-4.12597	-3.78814	0.337824	0.168912	-3.95706	-3.95706	3.957056
Configure5	-4.21355	-3.85886	0.354688	0.177344	-4.03621	-4.03621	4.036208
Configure6	-4.31582	-3.95787	0.357952	0.178976	-4.13685	-4.13685	4.136848
Configure7	-4.12597	-3.78814	0.337824	0.168912	-3.95706	-3.95706	3.957056
Configure8	-4.19098	-3.82269	0.368288	0.184144	-4.00683	-4.00683	4.006832
Configure9	-4.57803	-4.16269	0.415344	0.207672	-4.37036	-4.37036	4.37036
Configure10	-4.33541	-3.96086	0.374544	0.187272	-4.14814	-4.14814	4.148136

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	E_{HOMO}	E_{LUMO}	Eg	η	μ	E_{FL}	φ
SiCNT	-4.9865	-3.0507	1.9358	0.9679	-4.0186	-4.0186	4.0186
Configure1	-4.5247	-3.34043	1.18428	0.59214	-3.9325	-3.9325	3.9325
Configure2	-5.071	-2.9387	2.1327	1.0663	-4.0050	-4.0050	4.0050
Configure3	-5.3769	-2.8685	2.5084	1.2542	-4.1227	-4.1227	4.1227
Configure4	-4.9871	-3.0319	1.9551	0.9776	-4.0095	-4.0095	4.0095
Configure5	-4.9795	-3.0540	1.9255	0.9627	-4.0167	-4.0167	4.0167
Configure6	-5.2085	-3.0910	2.1175	1.0587	-4.1497	-4.1497	4.1497
Configure7	-4.8875	-2.9716	1.9159	0.9579	-3.9295	-3.9295	3.9295
Configure8	-5.0377	-3.0665	1.9712	0.9856	-4.0521	-4.0521	4.0521
Configure9	-5.4084	-3.0567	2.3517	1.1758	-4.2356	-4.2356	4.2356
Configure10	-5.0652	-3.1609	1.9043	0.9521	-4.1130	-4.1130	4.1130

Table S5 The geometrical parameters (bond lengths (R) is in Å), adsorption (E_{ad}) calculated at the CAM-B3LYP-D/6-31G* level

	SiCNT(7,0)	SiCNT (6,0)	CS_2-(7,0)SiCNT	CS_2-(6,0)SiCNT
C2-Si1	1.82546	1.77797	1.82392	1.80065
C8-Si7	1.82326	1.77742	1.82268	1.79939
C14-Si9	1.82409	1.77927	1.82372	1.80074
C6-Si5	1.76341	1.78844	1.76409	1.77632
C4-Si3	1.76503	1.78819	1.76553	1.77734
C10-Si11	1.76527	1.78961	1.76545	1.77845
C12-Si13	1.76390	1.78904	1.76427	1.77763
C=S	……	……	1.5504	1.55293
Ead			-25.1225	-27.0306

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C12-Si13	1.76390	1.78904	1.76427	1.77763
C=S	……	……	1.5504	1.55293
Ead			-25.1225	-27.0306