

Supporting Information

Spin-crossover complexes in nanoscale devices: main ingredients of the molecule-substrate interaction

Rocío Sánchez-de-Armas,^a Nicolas Montenegro,^{a,b} Aysegul Davelioglu,^c Enrique Burzurí^{c,d*} and Carmen J. Calzado^{a*}

^aDepartamento de Química Física. U. Sevilla, calle Prof. García González, s/n, 41012 Sevilla. Spain.

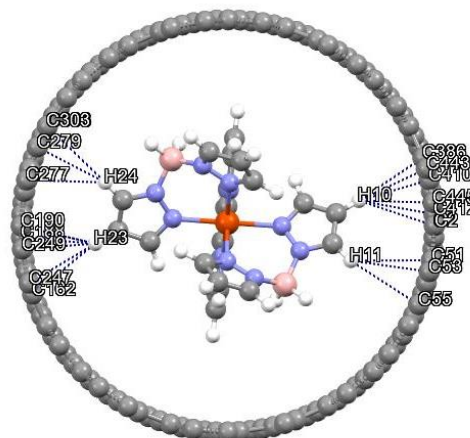
^bLaboratory of Theoretical Chemistry, Faculty of Chemistry and Biology, University of Santiago de Chile (USACH), 9170022, Santiago, Chile

^cIMDEA Nanociencia, Campus de Cantoblanco, Calle Faraday 9, 28049 Madrid, Spain.

^dDepartamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain.

geo2 HS

Atom1	Atom2	Length (Å)
C162	H23	3.330
C188	H23	3.337
C190	H23	3.091
C386	H10	3.159
C410	H10	3.318
C412	H10	3.325
C2	H10	3.247
C51	H11	3.392
C247	H23	3.202
C249	H23	3.117
C303	H24	3.312
C443	H10	3.195
C53	H11	3.264
C55	H11	3.377
C277	H24	3.215
C279	H24	3.175
C445	H10	3.276



geo2 LS

Atom1	Atom2	Length (Å)
C162	H22	3.124
C186	H22	3.348
C386	H19	3.208
C247	H22	3.364
C275	H23	3.249
C443	H19	3.357
C53	H20	3.378

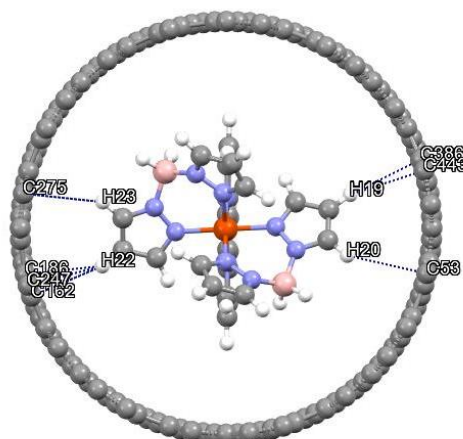
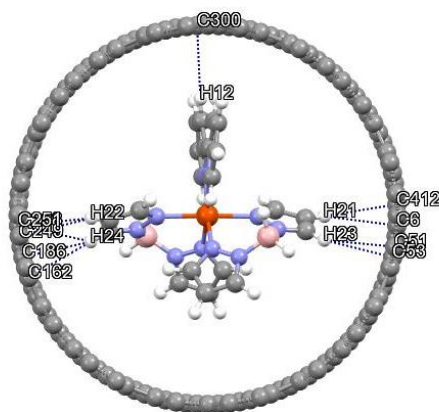


Figure S1 (cont.) Short contacts for SCO2@SWCNT

Molecule-nanotube contacts with distances ≤ 3.4 Å are reported

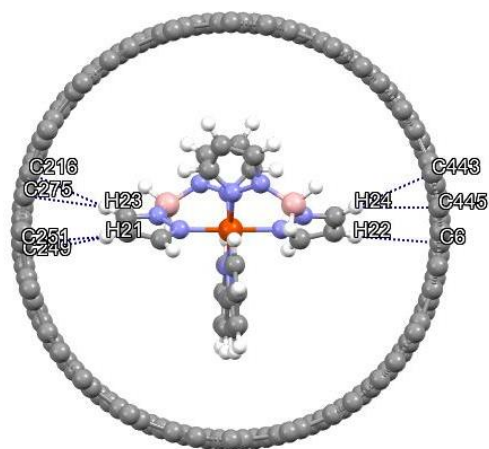
geo1 HS

Atom1	Atom2	Length (Å)
C6	H21	3.304
C51	H23	3.179
C53	H23	3.239
C162	H24	3.170
C186	H24	3.202
C188	H24	3.330
C249	H22	3.361
C251	H22	3.275
C300	H12	3.263
C412	H21	3.289



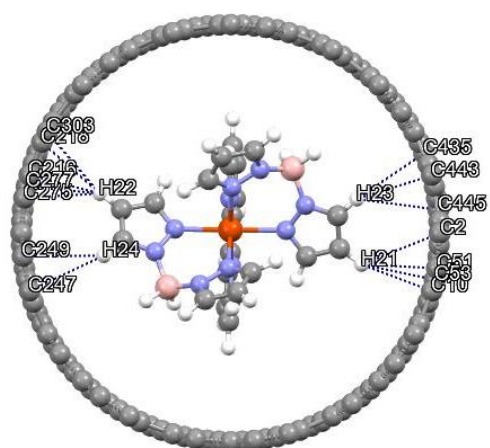
geo1 LS

Atom1	Atom2	Length (Å)
C6	H22	3.482
C216	H23	3.337
C249	H21	3.474
C251	H21	3.478
C275	H23	3.468
C443	H24	3.362
C445	H24	3.359



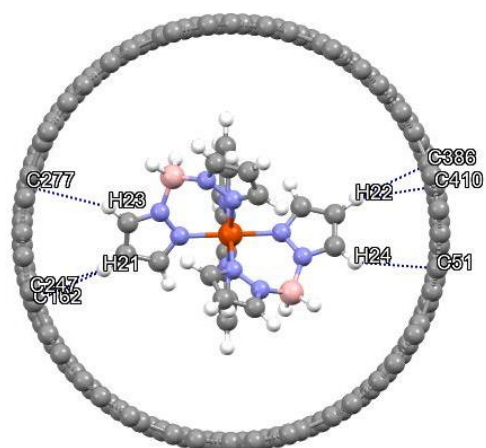
geo2 HS

Atom1	Atom2	Length (Å)
C10	H21	3.219
C51	H21	3.038
C53	H21	3.284
C216	H22	3.079
C218	H22	3.182
C249	H24	3.273
C275	H22	3.050
C443	H23	3.182



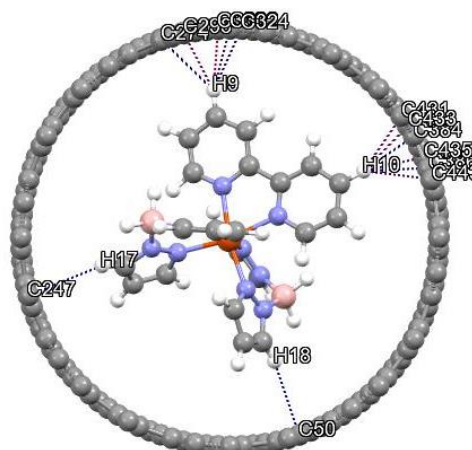
geo2 LS

Atom1	Atom2	Length (Å)
C51	H24	3.326
C162	H21	3.166
C247	H21	3.160
C277	H23	3.398
C386	H22	3.208
C410	H22	3.373



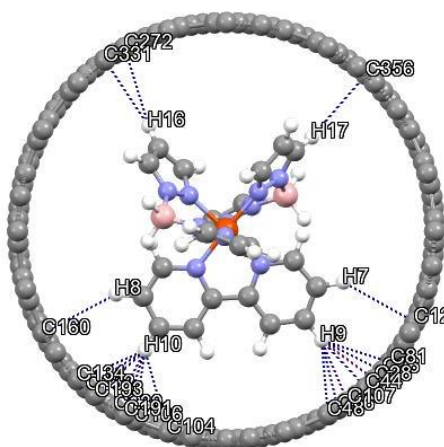
geo3 HS

Atom1	Atom2	Length (Å)
C50	H18	3.115
C247	H17	3.173
C274	H9	2.983
C298	H9	2.709
C300	H9	2.566
C302	H9	2.786
C324	H9	3.123
C384	H10	2.921
C386	H10	2.898
C431	H10	2.736
C433	H10	2.702
C435	H10	2.748
C443	H10	2.756



geo3 LS

Atom1	Atom2	Length (Å)
C12	H7	3.340
C26	H9	2.894
C28	H9	2.714
C44	H9	3.268
C46	H9	3.291
C48	H9	3.015
C81	H9	3.294
C104	H10	3.397
C106	H10	2.828
C107	H9	2.813
C130	H10	2.785
C132	H10	2.861
C134	H10	3.043
C160	H8	3.318
C191	H10	3.127
C193	H10	3.259
C272	H16	3.285
C331	H16	3.321
C356	H17	3.358



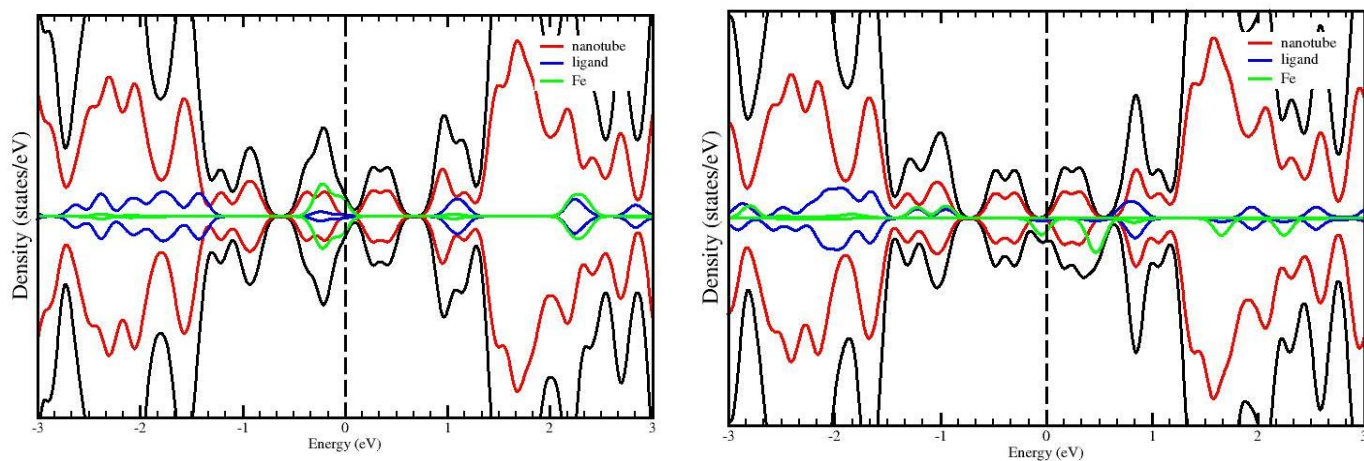


Figure S2. Density of states and projected density of states on Fe, ligands and nanotube for SCO1@SWCNT system (left) LS state, (right) HS state. Black lines correspond to the total density of states, while red, blue and green lines correspond to the density of states projected on the nanotube, ligands and Fe, respectively.

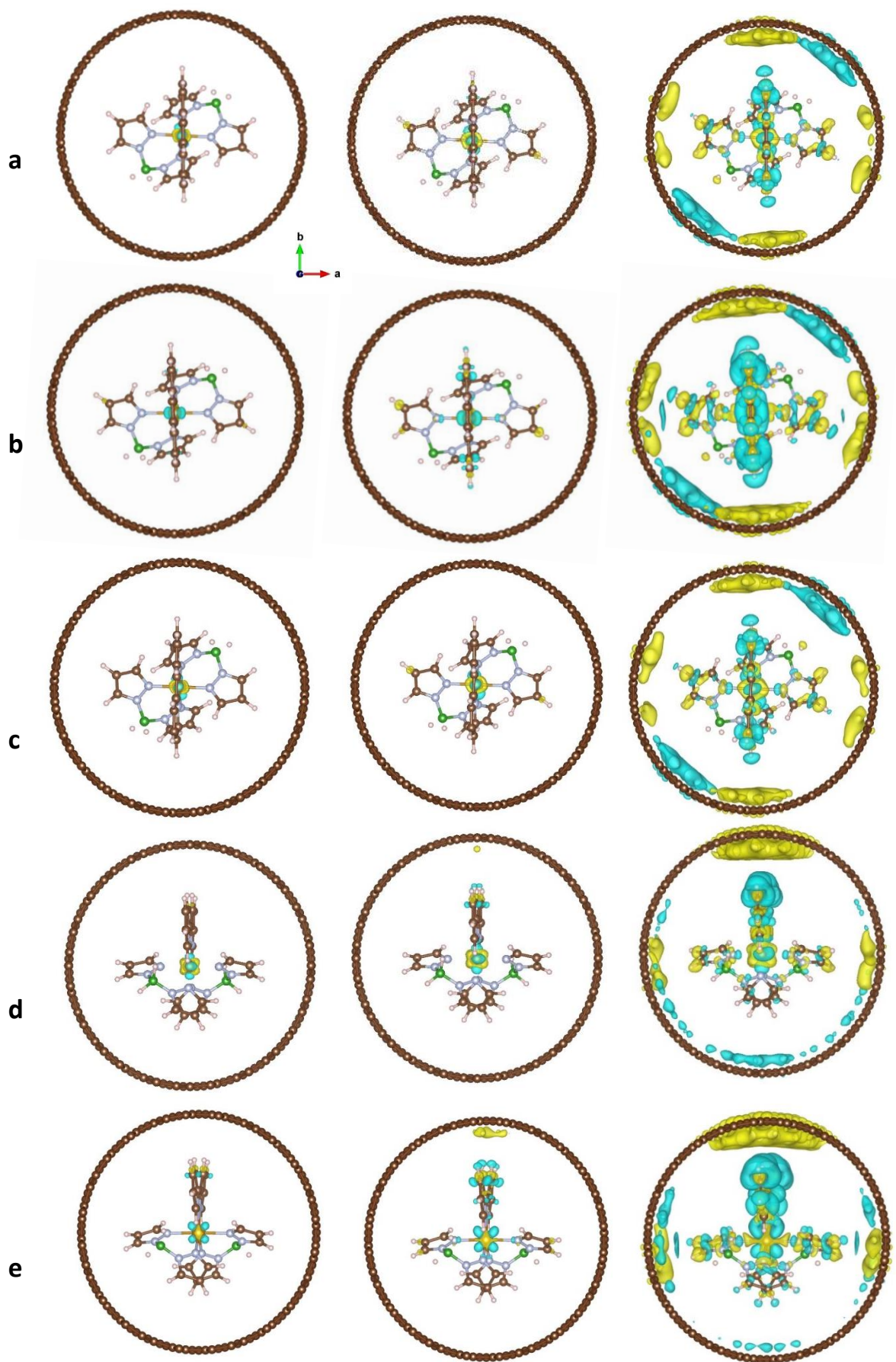


Figure S3. Plots of charge density difference, with isodensity values of (left) 10^{-3} e/bohr³, (middle) $5 \cdot 10^{-4}$ e/bohr³ and (right) 10^{-4} e/bohr³: (a) LS SCO1@SWCNT geo2, (b) HS SCO1@SWCNT geo2 (c) LS SCO2@SWCNT geo2, (d) LS SCO2@SWCNT geo1, (e) HS SCO2@SWCNT geo1.

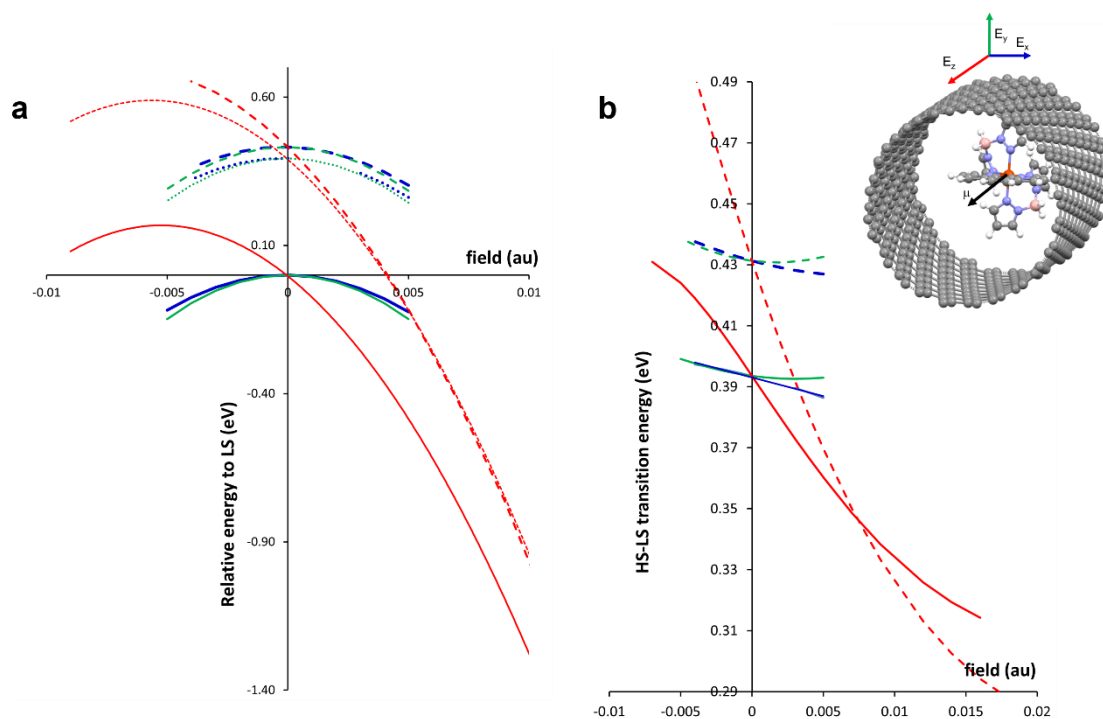


Figure S4. (a) Total energy (in eV) of the LS and HS states of SCO1 in presence of an external electric field (in au) along x (blue), y (green) or z (red) axis. Solid lines correspond to LS state, while dashed and dotted lines represent two thermally accessible HS states. (b) Impact of the applied electric field on the HS-LS transition energy (eV). Blue, green and red lines correspond to HS-LS energy under the influence of fields along x, y and z, respectively. The solid (dashed) lines correspond to the energy difference between the LS state and the lowest (excited) HS state in absence of field. The inset represents the optimal orientation of the encapsulated SCO1 complex, the black arrow is the electric dipole moment, and the blue, green and red arrows represent the electric fields along x, y and z axis, respectively.

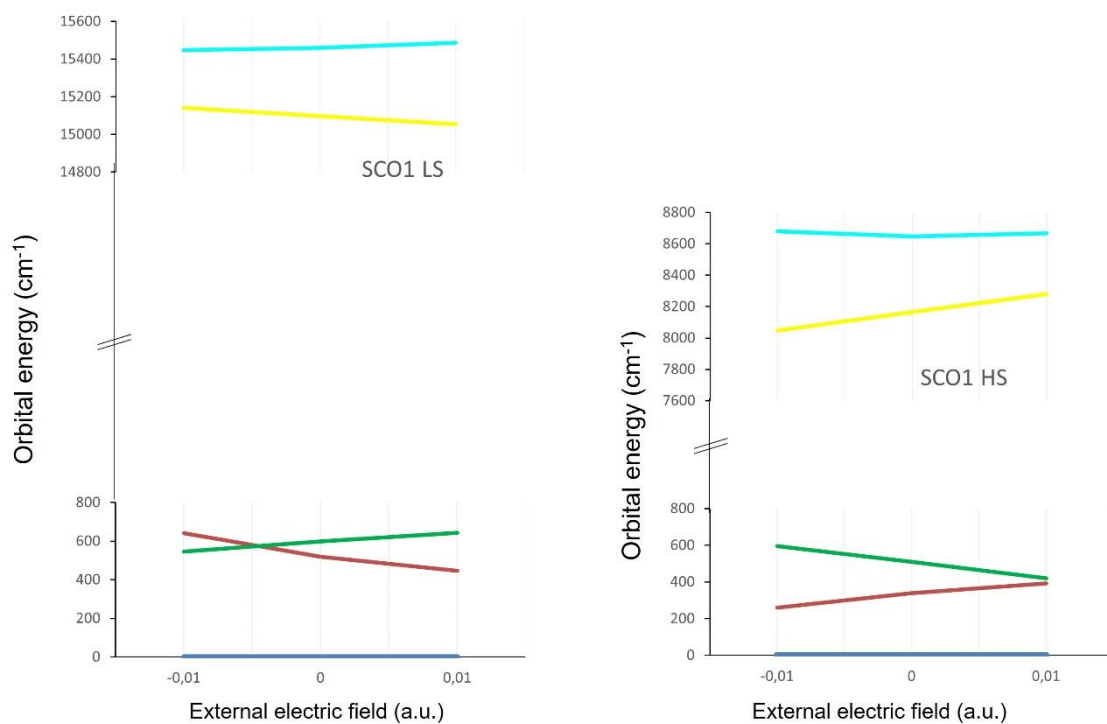


Figure S5. Impact of an external electric field applied along z axis (in atomic units) on the relative energies (cm⁻¹) of the Fe 3d t_{2g} (blue, red, and green lines) and e_g -like (cyan, yellow lines) orbitals for the LS and HS states of SCO1. All the calculations employ the optimized geometry of the encapsulated molecule (geo2).

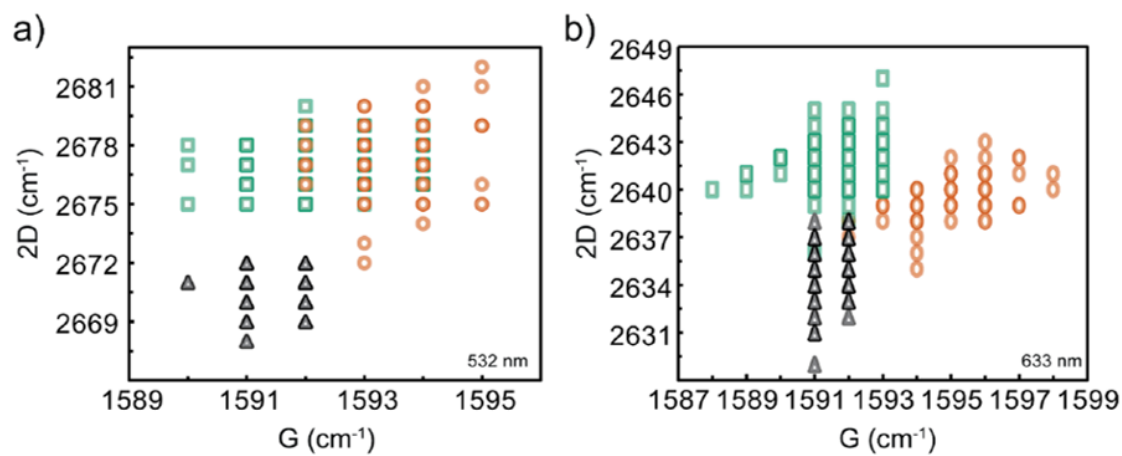


Figure S6. Plot of the Raman shift of 2D band vs G band for 100 different spectra ($\lambda=532$ nm and 633 nm) of open SWCNT (black triangles), SCO1@SWCNT (green squares) and SCO2@SWCNT (orange circles). Data points are shaded to indicate the frequency of occurrence

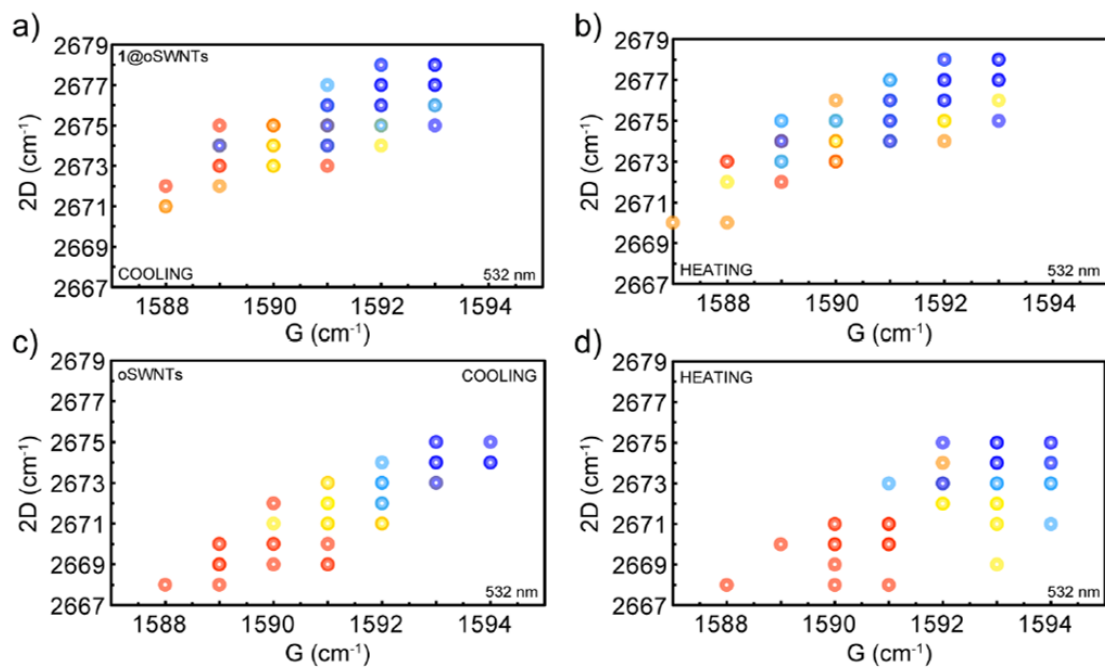


Figure S7. G-band displacement in SCO1@SWCNT while cooling (a) and heating (b) and for open SWCNT while cooling(c) and heating (d) for 532 nm laser. The different colours correspond to a temperature scale, from 273 K (red dots) to 153 K (dark blue dots) in intervals of 30 K (orange, yellow and pale blue). For each temperature, 20 different spectra are plotted.

Table S1. Fitting of the simulated LS and HS curves to an Arrhenius law for thermally activated electron transport.

$$\sigma/\tau = \frac{\sigma_0}{\tau} e^{(-\frac{B}{T})} + \frac{\sigma_i}{\tau}$$

	Spin state	σ_0/τ (1/(\Omega*cm*s))	B (K)	σ_i/τ (1/(\Omega*m*s))
No Doping	HS	3.57E+18	692.82	9.52E+14
	LS	6.53E+19	2733.64	-5.72E+13
Doping concentration (cm ⁻³)	Spin state	σ_0/τ (1/(\Omega*cm*s))	B (K)	σ_i/τ (1/(\Omega*m*s))
1.3 × 10 ⁻¹⁹	HS	2.88E+17	1824.59	7.17E+11
	LS	2.10E+18	2710.19	8.28E+10
1.47 × 10 ⁻¹⁹	HS	2.34E+18	2723.70	1.54E+12
	LS	2.03E+18	2666.20	7.28E+10
1.50 × 10 ⁻¹⁹	HS	1.68E+13	1907.47	-1.37E+08
	LS	5.19E+14	2797.94	-1.49E+07
Fermi level shift (eV)	Spin state	σ_0/τ (1/(\Omega*cm*s))	B (K)	σ_i/τ (1/(\Omega*m*s))
-0.135	HS	5.25E+18	2367.67	6.61E+11
	LS	7.65E+18	2774.40	1.36E+11
-0.155	HS	6.22E+18	2546.73	3.84E+11
	LS	5.43E+18	2552.44	4.36E+11
-0.164	HS	7.91E+18	2716.02	1.59E+11
	LS	4.55E+18	2371.14	7.57E+11

Table S2. The xyz coordinates of the most stable orientation of encapsulated SCO1 and SCO2 complexes. Due to the great length of the files, the rest of the optimized structures will be available on request.

SCO2@SWCNT: geo1 LS

507

C	41.644676	33.301273	0.000446
C	41.660015	33.301445	11.349944
C	41.645027	33.300667	3.782935
C	41.653591	33.299995	15.133245
C	41.630077	33.770046	2.432360
C	41.639477	33.770512	13.782486
C	41.443752	35.164059	2.161884
C	41.448746	35.163868	13.511526
C	41.331261	35.620182	0.811482
C	41.336983	35.619587	12.160805
C	40.842777	36.938789	0.540285
C	40.843140	36.936485	11.889983
C	41.634243	33.769508	6.214919
C	41.635941	33.769562	17.565470
C	41.594456	34.238338	4.864371
C	41.599060	34.237858	16.214750
C	41.329632	35.618889	4.593750
C	41.332329	35.618294	15.943701
C	41.191891	36.068035	3.243336
C	41.194290	36.067421	14.593064
C	40.628231	37.355492	2.972148
C	40.628216	37.353741	14.321837
C	40.391777	37.761375	1.621857
C	40.391109	37.758976	12.971457
C	39.548660	38.886784	1.350913
C	39.546753	38.883686	12.700587
C	39.225636	39.228218	0.000326
C	39.223160	39.224590	11.350300
C	41.602932	34.237995	8.647425
C	41.596867	34.238674	19.998224
C	41.536713	34.703056	7.296965
C	41.534863	34.703133	18.647282
C	41.193008	36.067139	7.026144
C	41.192524	36.067326	18.376253
C	41.026104	36.506485	5.675843
C	41.027245	36.505875	17.025679
C	40.387413	37.758282	5.404564
C	40.387482	37.757294	16.754009
C	40.128727	38.150276	4.053937
C	40.128132	38.148392	15.403416
C	39.222649	39.224812	3.782884
C	39.221348	39.222481	15.132422
C	38.882771	39.549538	2.432408
C	38.881191	39.546555	13.782015
C	37.757103	40.391781	2.160912
C	37.756489	40.390232	13.511267
C	37.351334	40.628716	0.810532
C	37.351219	40.628159	12.160927

C	36.064930	41.195309	0.539285
C	36.065422	41.196476	11.889778
C	41.543884	34.703823	11.079082
C	41.533554	34.703533	22.429729
C	41.452011	35.165680	9.728758
C	41.445812	35.166218	21.079220
C	41.032772	36.508072	9.457956
C	41.030987	36.509480	20.808277
C	40.841015	36.937305	8.107547
C	40.840775	36.938194	19.457449
C	40.129848	38.149895	7.836506
C	40.130127	38.150612	19.186052
C	39.846951	38.525639	6.486108
C	39.846661	38.524860	17.835382
C	38.882515	39.548641	6.214714
C	38.881889	39.547512	17.564192
C	38.522785	39.850449	4.864265
C	38.521980	39.848763	16.213665
C	37.352425	40.630077	4.592765
C	37.351868	40.628967	15.942894
C	36.933487	40.842754	3.242303
C	36.933334	40.842041	14.592564
C	35.616360	41.335331	2.971309
C	35.616428	41.336296	14.321681
C	35.160473	41.447689	1.620686
C	35.160915	41.450191	12.971205
C	33.766426	41.634472	1.350379
C	33.766727	41.638248	12.700429
C	33.296291	41.648842	22.699888
C	33.296173	41.656013	11.349537
C	40.630684	37.356201	10.539800
C	40.630512	37.358467	21.889997
C	39.851170	38.526924	10.268950
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C	39.547935	38.885777	8.918572
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C	38.525230	39.850861	19.996933
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C	36.504635	41.029980	20.807478
C	36.065357	41.196396	8.107035
C	36.064877	41.195980	19.457081
C	34.700684	41.539032	7.835720
C	34.700291	41.538116	19.186405
C	34.234398	41.601727	6.485020
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C	27.373827	39.215290	15.131863
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C	30.087883	41.033531	20.807478
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C	28.447868	40.125198	7.836528
C	28.447060	40.127987	19.185141
C	28.072409	39.841915	6.486121
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C	26.747179	38.516132	16.213192
C	25.966978	37.346626	4.592999
C	25.967081	37.345726	15.942251
C	25.754484	36.929165	3.242067
C	25.754320	36.925926	14.592010
C	25.260029	35.612965	2.971210
C	25.256567	35.610374	14.321355
C	25.146847	35.157516	1.620657
C	25.137098	35.154015	12.971184
C	24.958961	33.764160	1.349686
C	24.941019	33.760693	12.700839
C	24.941053	33.293953	22.699398
C	24.919106	33.290371	11.350078
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C	26.466167	38.143185	18.645834
C	25.753458	36.927559	7.025812
C	25.754330	36.930561	18.374971
C	25.561758	36.499634	5.675037
C	25.562267	36.500168	17.024876
C	25.141829	35.157093	5.403786
C	25.142860	35.157013	16.754175
C	25.055836	34.695919	4.052898
C	25.053633	34.694942	15.403864
C	24.942181	33.293633	3.781776
C	24.936609	33.292431	15.133260
C	24.958187	32.824375	2.431206
C	24.946466	32.821091	13.782887
C	25.147385	31.431374	2.160709
C	25.136209	31.428251	13.511693
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C	25.244909	30.971647	12.160648

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C	25.743322	29.655676	11.889893
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C	37.756012	26.211990	16.754187
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SCO1@SWCNT: geo2 LS

509

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