Supporting Information for:
Revealing the Adsorption Mechanisms of Nitroxides on Ultra-Pure, Metallicity-Sorted Carbon Nanotubes

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Contents
1 Samples S1
2 Simulated C Is Spectra S2
  2.1 Isolated Gas Phase Species . . . . . . . . . . . . . . . . . . S2
  2.2 Oxygen on SWCNTs . . . . . . . . . . . . . . . . . S2
3 Calculated Geometries and Total Energies S3
  3.1 Isolated Gas Phase Species . . . . . . . . . . . . . . . . . . S3
  3.2 NO_2+SWCNTs . . . . . . . . . . . . . . . . . . . S5
  3.3 O+SWCNTs . . . . . . . . . . . . . . . . . . . . . . . S8

1. Samples
The single-walled carbon nanotubes (SWCNTs) used in our experiments are material in which semiconducting and metallic separation has been achieved, allowing the formation of high-purity networks. S1 The overall morphology of these films can be observed in the scanning electron microscopy (SEM) micrograph shown in Fig. S1. This image corresponds to the semiconducting sample but there is no observable difference between both types of films with this imaging technique.

![Figure S1. Scanning Electron Microscopy micrograph at intermediate magnification showing the overall morphology of the nanotube films used in the experiments.](image)

Both types of samples were purified and separated into metallic and semiconducting tubes. They were then deposited on sapphire substrates. S2,S3 In our previous studies on these kinds of samples, we have shown that the SWCNT buckypapers have less than 1 wt% of processing residuals with X-ray photoelectron spectroscopy (XPS), with negligible residual magnetic metal impurity content. Typically, in these samples the remaining amount of surfactants, such as deoxycholate sodium salt, is below the detection limit of XPS and Fourier transform infrared spectroscopy (FT-IR). The G/D ratio in the Raman spectra of these SWCNT samples is typically around 20 from previous studies. S2,S3 As seen in the optical absorption spectra of these high purity samples (metal and semiconducting) shown in Fig. S2, no bands associated with the other conduction type are identified in either spectra.

Other spectroscopy studies that prove the high purity of the samples can be done with photoemission and X-ray absorption spectroscopy, and in particular valence band photoemission. These studies would be useless in the presence of impurities using a macroscopic sample, as can be understood from some previous publications. S4–S7

![Figure S2. Optical absorption spectra of the high purity samples: metallic (red) and semiconducting (blue).](image)
relative content of metallic to semiconducting SWCNTs is varied and quantum transport was achieved only in macroscopic networks of pure metallic SWCNTs.52

2. Simulated C 1s Spectra

Table S1. Carbon Species, Isolated Gas Phase Molecules, and Functional Groups Studied.

| C Species | Molecule | Formula | Group |
|-----------|----------|---------|-------|
| O=O       | carbon dioxide | CO₂     |       |
| C=O       | carbon monoxide | CO      |       |
| C≡O       | ethenone    | CH₂CO   | ketene |
|           | formaldehyde | CH₂O    | aldehyde/ carbonyl |
|           | acetyl radical | CH₃CO  | acety | ketone/carbonyl |
|           | acetone     | (CH₃)₂CO |       |
| C–O       | phenol      | C₆H₅OH  | hydroxyl |
|           | ethylene oxide | C₂H₄O  | epoxide |
| C–N       | nitrobenzene | C₆H₅NO₂ | nitro |
|           | pyridine-N-oxide | C₅H₅NO | amine oxide |
|           | pyridine    | C₅H₅N   | pyridyl |

2.1. Isolated Gas Phase Species. Core-level shifts provide an electronic “fingerprint” of the local chemical environment of an atomic species. This is due to the high degree of localization of these nearly-atomic levels, such as the C 1s. For this reason, simulated C 1s spectra for molecular species may be used to obtain a “blueprint” of the expected core-level shifts for various atomic species (C=O, C≡O, C–O, C–N) within representative functional groups (ketene, carbonyl, acetyl, hydroxyl, epoxide, nitro, amine oxide, pyridyl, etc.). Thus, to obtain further insight into the possible functional groups that may be present in the experimental SWCNT samples we have simulated the C 1s spectra for the representative molecules listed in Table S1 in gas phase.

To this end, we have employed more than 6 Å of vacuum and non-periodic boundary conditions in all directions. In this way, we ensure a common vacuum-level reference between the all-electron C 1s eigenenergies calculated for the various molecular species in Table S1. The C 1s spectra is then simulated by employing a Lorentzian broadening with an inverse lifetime of 0.27 eV, and aligning the calculated and experimental C 1s levels of the C–C species in acetone, as shown in Fig. S3.

Comparison of the simulated C 1s spectra in Fig. S3 with the high binding energy feature in the XPS C 1s spectra for SWCNTs dosed with NO₂ clearly indicates this feature is due to a C=O species, as both C–O and C–N shifts are too small. Further, the core-level shift arising from a ketene group yields the largest shift, and is well separated from the carbonyl and acetyl groups. This provides further verification that this feature observed in the XPS C 1s spectra is due to a C=O species in a ketene group on a SWCNT. Furthermore, the good matching shown in Fig. S3 between calculated and experimental XPS spectra for acetone (red squares)58 validates our computational approach.

2.2. Oxygen on SWCNTs. To further justify our assignment of the feature observed in the XPS C 1s spectra at high binding energy to the C=O species of a ketene group, we have performed further calculations for the C=O species of a carbonyl group and C–O species of epoxide and chemisorbed O₂. Since core states are highly localized, we can investigate the effect of several functional groups within the same calculation. In this way, we can ensure a common reference between calculations. The optimized geometries, C 1s levels, and simulated spectra for a carbonyl group adsorbed on a carbene site of a monovacancy, an epoxide group adsorbed on a pentagon adjacent to a monovacancy, and an O₂ molecule adsorbed on a semiconducting (10,0) and metallic (6,6) SWCNT are shown in Fig. S4. For both types of SWCNT, we find the C=O species of a carbonyl group and C–O species are at too weak binding energy to give rise to the experimentally observed feature. However, it should be noted that the presence of carboxyl and epoxide groups in the experimental spectra cannot be ruled out as their signals may appear in the region between the main and ketene peaks.
3. Calculated Geometries and Total Energies

All geometries were optimized within the local density approximation (LDA)\textsuperscript{S9} until a maximum force less than 0.05 eV/Å was obtained. The total energy for the relaxed structure is given in Hartrees. All coordinates (provided in xyz format below) and cell dimensions are given in Å. For the acetone molecule, we also provide the experimental geometry and its corresponding LDA energy in Table S8.

3.1. Isolated Gas Phase Species.

Table S2. Coordinates in Å of carbon dioxide

| Energy     | Cell Dimensions         | C         | O         | H         |
|------------|-------------------------|-----------|-----------|-----------|
| $E = -188.4210$ Ha | carbon dioxide cell=[12.8, 12.8, 14.4] | 6.400000 6.400000 7.200000 | O 6.400000 6.400000 8.376975 | O 6.400000 6.400000 6.023025 |

Table S3. Coordinates in Å of carbon monoxide

| Energy     | Cell Dimensions         | C         | O         | H         |
|------------|-------------------------|-----------|-----------|-----------|
| $E = -113.0620$ Ha | carbon monoxide cell=[12.8, 12.8, 13.6] | 6.400000 6.400000 7.339014 | O 6.400000 6.400000 6.205357 |

Table S4. Coordinates in Å of ethene

| Energy     | Cell Dimensions         | C         | O         | H         |
|------------|-------------------------|-----------|-----------|-----------|
| $E = -152.0299$ Ha | ethene cell=[14.4, 14.5, 12.8] | 7.200000 6.629969 6.400000 | O 7.200000 9.109202 6.400000 | H 8.145708 6.091162 6.400000 | H 6.254292 6.091162 6.400000 | C 7.200000 7.937511 6.400000 |

Table S5. Coordinates in Å of formaldehyde

| Energy     | Cell Dimensions         | C         | O         | H         |
|------------|-------------------------|-----------|-----------|-----------|
| $E = -114.2274$ Ha | formaldehyde cell=[14.4, 14.4, 12.8] | 7.200000 6.886825 6.400000 | O 7.200000 8.099027 6.400000 | H 8.153556 6.298014 6.400000 | C 7.200000 7.937511 6.400000 |

Table S6. Coordinates in Å of acetyl radical

| Energy     | Cell Dimensions         | C         | O         | H         | C         |
|------------|-------------------------|-----------|-----------|-----------|-----------|
| $E = -152.5804$ Ha | acetyl radical cell=[14.4, 13.6, 15.2] | 7.186157 6.658713 9.023855 | O 7.192034 5.998570 8.033677 | C 7.191491 6.400000 6.620282 | C 7.190326 7.545179 6.553618 | H 6.305273 6.023357 6.120142 | H 8.075547 6.018981 6.121409 |

Table S7. Coordinates in Å of acetone

| Energy     | Cell Dimensions         | C         | O         | H         | C         |
|------------|-------------------------|-----------|-----------|-----------|-----------|
| $E = -192.2195$ Ha | acetone cell=[14.4, 16.8, 15.2] | 7.194479 8.388653 9.005765 | O 7.197208 8.395448 7.781195 | C 7.195155 9.660136 6.987924 | H 7.191535 10.535616 7.648972 | H 6.312782 9.689635 6.326095 | H 8.072519 9.697749 6.320201 | C 7.197111 7.139395 6.975212 | H 6.336770 7.128990 6.284221 | H 7.164178 6.254868 7.622547 | H 8.094251 7.099335 6.334092 |

Table S8. Experimental coordinates in Å of acetone

| Energy     | Cell Dimensions         | C         | O         | H         | C         |
|------------|-------------------------|-----------|-----------|-----------|-----------|
| $E = -192.2169$ Ha | acetone cell=[14.4, 16.8, 15.2] | 7.310400 9.394500 6.841100 | C 7.491400 8.438600 8.012200 | C 7.346500 6.949100 7.732400 | O 7.744600 8.853300 9.139900 | H 6.308700 9.296400 6.423600 | H 8.039000 9.179100 6.060100 | H 7.448600 10.425900 7.166300 | H 6.354100 6.732400 7.338200 | H 8.091300 6.626100 7.005600 | C 7.486600 6.374100 8.648000 |
### Table S9. Coordinates in Å of nitrobenzene

\[E = -434.6593 \text{ Ha}\]

|        |        |        |         |         |
|--------|--------|--------|---------|---------|
|        |        |        |         |         |
|        |        |        |         |         |
|        |        |        |         |         |

\[\text{nitrobenzene cell} = [17.6, 18.4, 12.8]\]

- C 9.423058 11.092330 6.400000
- C 10.196996 9.942475 6.400000
- C 9.587988 8.700289 6.400000
- C 8.206024 8.641131 6.400000
- C 7.417426 9.778537 6.400000
- C 8.037533 11.011347 6.400000
- N 7.560735 7.345418 6.400000
- O 8.294843 6.333715 6.400000
- O 6.311257 7.317178 6.400000
- H 9.913310 12.069673 6.400000
- H 11.288687 10.008559 6.400000
- H 10.149964 7.762432 6.400000
- H 6.332306 9.665477 6.400000
- H 7.442444 11.927286 6.400000

### Table S10. Coordinates in Å of phenol

\[E = -305.6367 \text{ Ha}\]

|        |        |        |         |         |
|--------|--------|--------|---------|---------|
|        |        |        |         |         |
|        |        |        |         |         |
|        |        |        |         |         |

\[\text{phenol cell} = [17.6, 12.8, 16.8]\]

- H 10.321216 6.457342 10.546109
- C 9.781573 6.420628 9.596916
- C 10.476565 6.404482 8.400232
- H 11.567680 6.415058 8.399552
- C 9.778830 6.382661 7.202859
- H 10.149964 7.762432 6.400000
- H 6.332306 9.665477 6.400000
- H 7.442444 11.927286 6.400000

### Table S11. Coordinates in Å of pyridine-N-oxide

\[E = -321.5779 \text{ Ha}\]

|        |        |        |         |         |
|--------|--------|--------|---------|---------|
|        |        |        |         |         |
|        |        |        |         |         |
|        |        |        |         |         |

\[\text{pyridine-N-oxide cell} = [17.6, 16.8, 12.8]\]

- C 10.227455 8.422011 6.399837
- C 9.570291 7.219522 6.401303
- C 8.185029 7.184543 6.401162
- C 7.505801 8.392385 6.400469
- C 8.191833 9.579328 6.399165
- N 9.553038 9.600006 6.398242
- O 10.183576 10.734746 6.396520
- O 11.311465 8.542908 6.40213
- H 10.157848 6.299433 6.404773
- H 7.643538 6.237603 6.403748
- H 6.413689 8.424233 6.402278
- H 7.735051 10.569441 6.398282

### Table S12. Coordinates in Å of ethylene oxide

\[E = -153.1918 \text{ Ha}\]

|        |        |        |         |         |
|--------|--------|--------|---------|---------|
|        |        |        |         |         |
|        |        |        |         |         |
|        |        |        |         |         |

\[\text{ethylene oxide cell} = [15.2, 14.4, 13.6]\]

- C 6.871610 7.204511 6.290753
- O 7.598001 7.232259 7.548895
- H 6.338607 6.269248 6.085070
- H 6.334459 8.129167 6.051221
- H 8.862771 6.269634 6.093454
- H 8.865648 8.130823 6.059390
- C 8.328846 7.205117 6.294901

### Table S13. Coordinates in Å of pyridine

\[E = -246.3191 \text{ Ha}\]

|        |        |        |         |         |
|--------|--------|--------|---------|---------|
|        |        |        |         |         |
|        |        |        |         |         |
|        |        |        |         |         |

\[\text{pyridine cell} = [17.6, 16.8, 12.8]\]

- C 10.154700 8.430686 6.400000
- C 9.506548 7.207144 6.400000
- C 8.123921 7.196973 6.400000
- C 7.443965 8.403151 6.400000
- C 8.186882 9.574961 6.400000
- N 9.514442 9.595633 6.400000
- H 11.248960 8.479876 6.400000
- H 10.079243 6.276600 6.400000
- H 7.573236 6.251999 6.400000
- H 6.351508 8.439459 6.400000
- H 7.679768 10.548184 6.400000
### 3.2. NO$_2$+SWCNTs.

Table S14. Coordinates in Å of 10NO$_2$+(10,0) SWCNT

$E = -5063.4424$ Ha

| Coordinates | 10NO$_2$+(10,0)SWCNT cell=[18.4, 18.4, 8.526] | C | 9.101634 | 13.091229 | 5.652072 |
|-------------|-----------------------------------------------|---|----------|-----------|-----------|
|             |                                               | C | 7.900159 | 12.868088 | 4.965212  |
|             |                                               | C | 7.882133 | 12.864111 | 7.817982  |
|             |                                               | C | 6.827448 | 12.306216 | 7.115345  |
|             |                                               | C | 6.818022 | 12.290757 | 5.686636  |
|             |                                               | C | 5.953511 | 11.467949 | 4.976535  |
|             |                                               | C | 5.934792 | 11.436007 | 7.831855  |
|             |                                               | C | 5.387354 | 10.360430 | 7.131935  |
|             |                                               | C | 5.166130 | 10.427797 | 5.676324  |
|             |                                               | C | 5.254975 | 9.129872  | 4.965696  |
|             |                                               | C | 5.245707 | 9.145068  | 7.815926  |
|             |                                               | C | 5.490058 | 7.943472  | 7.094698  |
|             |                                               | C | 5.491330 | 7.961861  | 5.665606  |
|             |                                               | C | 6.077578 | 6.861285  | 4.949240  |
|             |                                               | C | 6.026228 | 6.876282  | 7.800385  |
|             |                                               | C | 6.796761 | 5.829978  | 7.096988  |
|             |                                               | C | 6.934674 | 6.018236  | 5.648983  |
|             |                                               | C | 8.055422 | 5.504585  | 4.965769  |
|             |                                               | C | 8.040330 | 5.504404  | 7.812355  |
|             |                                               | C | 9.237887 | 5.352943  | 7.112836  |
|             |                                               | C | 9.253856 | 5.317288  | 5.690602  |
|             |                                               | C | 10.465774 | 5.510267 | 4.979698  |
|             |                                               | C | 10.455168 | 5.513935 | 7.841034  |
|             |                                               | C | 11.687666 | 5.905013 | 7.127931  |
|             |                                               | C | 11.57224 | 6.061908  | 5.672466  |
|             |                                               | C | 12.381882 | 6.948402 | 4.980064  |
|             |                                               | C | 12.401124 | 6.986174 | 7.832658  |
|             |                                               | C | 12.924725 | 8.057201 | 7.122157  |
|             |                                               | C | 12.907855 | 8.067445 | 5.659589  |
|             |                                               | C | 13.107473 | 9.238725 | 4.984472  |
|             |                                               | N | 9.050969 | 14.991482 | 7.167179  |
|             |                                               | O | 10.127217 | 15.529337 | 7.071566  |
|             |                                               | O | 9.791927 | 15.480055 | 7.251743  |
|             |                                               | N | 12.540348 | 13.941142 | 2.928208  |
|             |                                               | O | 13.721240 | 13.715673 | 3.018993  |
|             |                                               | O | 11.964697 | 14.997316 | 2.843685  |
|             |                                               | N | 14.661701 | 11.136631 | 5.556480  |
|             |                                               | O | 15.529008 | 10.304072 | 5.439924  |
|             |                                               | O | 14.759807 | 12.336267 | 5.630089  |
|             |                                               | C | 12.729488 | 4.571236 | 7.223681  |
|             |                                               | C | 12.187426 | 3.496533 | 7.293900  |
|             |                                               | O | 13.902903 | 4.841264 | 7.174470  |
|             |                                               | N | 14.791341 | 7.433008 | 1.340846  |
|             |                                               | O | 14.923683 | 6.237818 | 1.267897  |
|             |                                               | O | 15.629148 | 8.295844 | 1.397425  |
|             |                                               | N | 9.220716 | 3.390945 | 1.325045  |
|             |                                               | C | 8.145471 | 2.896902 | 1.547391  |
|             |                                               | O | 10.281705 | 2.870663 | 1.094029  |
|             |                                               | N | 5.813488 | 4.429131 | 7.171326  |
|             |                                               | O | 4.673776 | 4.598514 | 8.617428  |
|             |                                               | O | 6.360241 | 3.426187 | 7.552793  |
|             |                                               | N | 3.643512 | 7.304326 | 2.952321  |
|             |                                               | O | 2.80813 | 8.166220 | 2.971389  |
|             |                                               | O | 3.513974 | 6.105191 | 2.962416  |
|             |                                               | N | 3.576094 | 10.893697 | 5.590000  |
|             |                                               | C | 3.386427 | 12.085325 | 5.519854  |
|             |                                               | C | 2.770852 | 9.995532 | 5.652510  |
|             |                                               | N | 5.680725 | 13.873047 | 1.336841  |

C: Carbon, O: Oxygen, N: Nitrogen
Table S15. Coordinates in Å of 12NO2+(6,6) SWCNT

\[ E = -6076.6786 \text{ Ha} \]

| 132 | 12NO2+(6,6)SWCNT cell=[23.2, 23.2, 9.845] | C | 13.292307 9.133371 1.855637 |
| 13 | C | 13.074585 10.528222 1.853716 |
| 10 | C | 12.790702 11.177528 0.623966 |
| 7 | C | 11.901133 12.277924 0.622594 |
| 5 | C | 11.323747 12.688151 1.853863 |
| 4 | C | 10.002506 13.188566 1.854595 |
| 3 | C | 9.297836 13.271190 0.622976 |
| 1 | C | 7.902139 13.041768 0.624096 |
| 2 | C | 7.253976 12.75461 1.854855 |
| 1 | C | 6.148872 11.876000 1.856060 |
| 2 | C | 5.730489 11.304742 0.625870 |
| 1 | C | 5.229376 9.983384 0.627148 |
| 1 | C | 5.163176 9.279158 1.858609 |
| 5 | C | 5.397728 7.886933 1.859530 |
| 4 | C | 5.680371 7.236031 0.628226 |
| 3 | C | 6.577626 6.143123 0.629573 |
| 2 | C | 7.147993 5.724059 1.859627 |
| 1 | C | 8.463016 5.207268 1.859172 |
| 1 | C | 9.167857 5.131332 0.629026 |
| 1 | C | 10.563943 5.639718 1.858668 |
| 1 | C | 11.203952 6.532476 1.857865 |
| 1 | C | 12.730195 7.102584 0.625631 |
| 1 | C | 13.216479 8.431812 0.625796 |
| 1 | C | 13.292292 9.133611 4.317576 |
| 1 | C | 13.075034 10.528222 4.316932 |
| 1 | C | 12.799053 11.183371 3.084384 |
| 1 | C | 11.896914 12.274291 3.083413 |
| 1 | C | 11.323512 12.686343 4.313469 |
| 1 | C | 10.001930 13.181580 4.312880 |
| 1 | C | 9.297924 13.259725 3.084199 |
| 1 | C | 7.900107 13.042571 3.085436 |
| 1 | C | 7.252805 12.754233 4.316740 |
| 1 | C | 6.144598 11.877375 4.317409 |
| 1 | C | 5.724846 11.307504 3.086416 |
| 1 | C | 5.228903 9.983686 3.088341 |
| 1 | C | 5.164614 9.279145 4.318883 |
| 1 | C | 5.399963 7.886916 4.318640 |
| 1 | C | 5.68035 7.240427 3.089053 |
| 1 | C | 6.575956 6.139718 4.321380 |
| 1 | C | 7.148128 5.722781 3.089450 |
| 1 | C | 8.46154 5.206461 3.089862 |
| 1 | C | 9.167246 5.121614 3.089862 |
| 1 | C | 10.563337 5.346817 3.088639 |
| 1 | C | 11.209076 5.639055 4.318317 |
| 1 | C | 12.301544 6.533188 4.315613 |
| 1 | C | 12.719768 7.106544 3.086656 |
| 1 | C | 13.224584 8.428017 3.087150 |
| 1 | C | 13.292546 9.133442 6.777681 |
| 1 | C | 13.074492 10.528177 6.776227 |
| 1 | C | 12.789737 11.177066 5.546327 |
| 1 | C | 11.901076 12.276825 5.544966 |
| 1 | C | 11.323609 12.686401 6.776402 |
### 3.3. O+SWCNTs.

| Table S16. Coordinates in Å of O+(10,0) SWCNT ketene group |
|---------------------------------------------------------------|
| $E = -6125.6211$ Ha |

| C    | 7.745553 5.858140 5.653574 |
| C    | 8.953066 5.648642 4.939097 |
| C    | 8.948815 5.642618 7.783193 |
| C    | 10.162505 5.823984 7.070629 |
| C    | 10.164617 5.828317 5.653251 |
| C    | 11.273822 6.344432 4.940068 |
| C    | 11.273511 6.340353 7.788179 |
| C    | 12.205227 7.141418 7.078873 |
| C    | 12.211458 7.137350 5.657170 |
| C    | 12.898776 8.149527 4.939290 |
| C    | 12.874032 8.168045 7.797979 |
| C    | 13.250373 9.328086 7.072079 |
| C    | 13.265470 9.318691 5.657335 |
| C    | 13.272612 10.541312 4.943742 |
| C    | 13.255264 10.560227 7.769273 |
| C    | 12.903883 11.725988 7.048716 |
| C    | 12.892021 11.711217 5.646356 |
| C    | 12.122769 12.673792 4.935991 |
| C    | 12.168274 12.728800 7.754177 |
| C    | 11.072019 13.307126 7.049798 |
| C    | 11.059134 13.294285 5.647272 |
| C    | 9.846815 13.501048 4.944514 |
| C    | 9.868695 13.484160 7.771675 |
| C    | 8.649395 13.307763 7.073426 |
| C    | 8.637720 13.322382 5.658562 |
| C    | 7.525390 12.807121 4.947123 |
| C    | 7.543831 12.782226 7.798892 |
| C    | 6.609895 11.994939 7.080459 |
| C    | 6.603452 12.002868 5.658985 |
| C    | 5.925811 10.983788 4.940961 |
| C    | 12.713269 8.264622 12.049774 |
| C    | 13.052311 9.437366 11.342922 |
| C    | 13.163381 9.384759 9.929570 |
| C    | 13.229806 10.580008 9.182998 |
| C    | 12.989012 10.681896 12.049160 |
| C    | 12.959853 11.833462 11.256221 |
| C    | 12.958611 11.786886 9.860630 |
| C    | 12.223335 12.789257 9.140203 |
| C    | 12.517048 13.126814 11.787236 |
| C    | 11.172807 13.381562 11.261265 |
| C    | 11.125178 13.368545 9.864936 |
| C    | 9.891915 13.460864 9.186428 |
| C    | 10.025487 13.241168 12.044772 |
| C    | 8.783110 13.126443 11.345522 |
| C    | 8.716422 12.228197 9.931260 |
| C    | 7.577257 12.750030 9.217546 |
| C    | 7.663383 12.637554 12.051717 |
| C    | 6.672895 11.923858 11.340816 |
| C    | 6.647878 11.951966 9.923897 |
| C    | 5.930900 10.962198 9.205824 |
| C    | 5.942774 10.941224 12.051946 |
| C    | 5.533410 9.790966 11.333618 |
| C    | 5.538902 9.798438 9.916190 |
| C    | 5.520832 8.577257 9.199808 |
| C    | 5.503493 8.566539 12.048757 |
| C    | 5.897929 7.407486 11.331122 |
| C    | 5.903338 7.412792 9.915245 |
| C    | 6.677823 6.463438 9.198984 |
Table S17. Coordinates in Å of O+(6,6) SWCNT ketene group

\[ E = -6428.1889 \text{ Ha} \]

| C   | 6.671946 | 6.457200 | 12.049055 |
| C   | 7.731534 | 5.841612 | 11.331802 |
| C   | 7.735482 | 5.845930 | 9.915545  |
| C   | 8.943552 | 5.636419 | 9.200600  |
| C   | 8.936753 | 5.623090 | 12.048098 |
| C   | 10.146600| 5.809108 | 11.332649 |
| C   | 10.153107| 5.814615 | 9.915181  |
| C   | 11.263097| 6.341925 | 9.204694  |
| C   | 11.240222| 6.352838 | 12.050595 |
| C   | 12.128440| 7.193783 | 11.338686 |
| C   | 12.160275| 7.171739 | 9.922169  |
| C   | 12.838688| 8.192459 | 9.216510  |
| C   | 12.827549| 8.202331 | 16.298281 |
| C   | 13.131649| 9.390627 | 15.586476 |
| C   | 12.993612| 9.475211 | 14.176398 |
| C   | 12.808841| 10.718801| 13.478433 |
| C   | 13.237488| 10.587071| 16.321986 |
| C   | 12.802588| 11.738015| 15.650705 |
| C   | 12.360942| 11.805653| 14.301651 |
| C   | 12.157633| 12.714714| 16.427003 |
| C   | 11.094374| 13.206144| 15.653148 |
| C   | 11.225565| 12.781914| 14.302960 |
| C   | 10.083985| 13.066510| 13.481757 |
| C   | 9.892819 | 13.467037| 16.324836 |
| C   | 8.722392 | 13.196340| 15.589896 |
| C   | 8.825440 | 13.072763| 14.179313 |
| C   | 7.677572 | 12.639824| 13.463682 |
| C   | 7.582250 | 12.742809| 16.300318 |
| C   | 6.650790 | 11.947982| 15.592783 |
| C   | 5.946677 | 10.943479| 13.465493 |
| C   | 5.933582 | 10.960602| 16.310106 |
| C   | 5.541632 | 9.797063 | 15.598543 |
| C   | 5.536475 | 9.792041 | 14.181702 |
| C   | 5.504109 | 8.567229 | 13.466097 |
| C   | 5.520756 | 8.576299 | 16.315788 |
| C   | 5.902159 | 7.411897 | 15.599297 |
| C   | 5.896860 | 7.407483 | 14.183460 |
| C   | 6.672337 | 6.458074 | 13.465777 |
| C   | 6.675767 | 6.461909 | 16.315565 |
| C   | 7.734783 | 5.847201 | 15.598985 |
| C   | 7.732632 | 5.844001 | 14.182607 |
| C   | 8.937635 | 5.626141 | 13.465719 |
| C   | 8.942273 | 5.639015 | 13.314616 |
| C   | 10.150333| 5.821299 | 15.598423 |
| C   | 10.147286| 5.816144 | 14.181092 |
| C   | 11.242116| 6.358983 | 13.464259 |
| C   | 11.257708| 6.351664 | 16.309966 |
| C   | 12.152929| 7.180070 | 15.591739 |
| C   | 12.131832| 7.203479 | 14.175330 |
| C   | 12.713355| 8.279373 | 13.461236 |
| O   | 13.281143| 13.925435| 12.480613 |
| O   | 13.974502| 14.600021| 13.133535 |

O+(6,6)SWCNT cell: [19.2, 19.2, 17.2287]
| Number | Coordinates in Å of O2@MV (carbonyl and epoxy groups) and O2++(10,0) SWCNT |
|--------|--------------------------------------------------------------------------------|
| C      | 7.738806 5.843763 7.081471 |
| C      | 7.729351 5.836085 5.680856 |
| C      | 8.913891 5.752018 4.954921 |
| C      | 8.951809 5.672611 7.788454 |
| C      | 10.156523 5.859771 7.069170 |
| C      | 10.140450 5.899717 5.655041 |
| C      | 11.264836 6.392391 4.941276 |
| C      | 11.281988 6.315295 7.789581 |
| C      | 12.215691 7.146768 7.082404 |
| C      | 12.219615 7.148911 5.685527 |
| C      | 12.920043 8.154761 4.940198 |
| C      | 12.890942 8.169215 7.803115 |
| C      | 13.264065 9.331971 7.077451 |
| C      | 13.280660 9.323563 5.660265 |
| C      | 13.283737 10.544557 4.946109 |
| C      | 13.266842 10.562554 7.773084 |
| C      | 12.906862 11.728190 7.045891 |
| C      | 12.896945 11.714529 5.650505 |
| C      | 12.116940 12.672941 4.933812 |
| C      | 12.158069 12.720427 7.725759 |
| C      | 11.061279 13.298873 7.049669 |
| C      | 11.049601 13.286513 5.640785 |
| C      | 9.840141 13.507460 4.945319 |
| C      | 9.860672 13.486660 7.773659 |
| C      | 8.638737 13.327774 7.076734 |
| C      | 8.628129 13.347030 5.662339 |
| C      | 7.515193 12.833896 4.943333 |
| C      | 7.534742 12.803531 7.804394 |
| C      | 6.607437 12.062665 7.083471 |
| C      | 6.610398 12.010655 5.659973 |
| C      | 5.975197 10.968364 4.942202 |
| C      | 5.489657 5.072413 3.504483 |
| C      | 5.494154 5.079922 4.976442 |
| C      | 12.710235 8.272018 12.052568 |
| C      | 13.056495 9.439530 11.343147 |
| C      | 13.170049 9.388068 9.929377 |
| C      | 13.242717 10.583474 9.185814 |
| C      | 13.015115 10.686907 12.041169 |
| C      | 12.976722 11.850618 11.252406 |
| C      | 12.960192 11.793675 9.865016 |
| C      | 12.208698 12.779135 9.135638 |
| C      | 12.523917 13.151997 11.789493 |
| C      | 11.157788 13.339562 11.265154 |
| C      | 11.113446 13.341983 9.864008 |
| C      | 9.882596 13.457912 9.190187 |
| C      | 10.018458 13.203401 12.047703 |
| C      | 8.775356 13.104095 11.350517 |
| C      | 8.707116 13.225211 9.937393 |
| C      | 7.561657 12.761591 9.222592 |
| C      | 7.648668 12.624422 12.055428 |
| C      | 6.649326 11.926864 11.342344 |
| C      | 6.629133 11.962744 9.924391 |
| C      | 5.915533 10.973031 9.203312 |
| C      | 5.908581 10.952877 12.053596 |
| C      | 5.520026 9.796382 11.331891 |
| C      | 5.529886 9.802931 9.915917 |
| C      | 5.562688 8.580530 9.204110 |
| C      | 5.502476 8.572888 12.047531 |
Table S19. Coordinates in Å of 2O@MV (carbonyl and epoxy groups) and O$_2^+$ (6,6) SWCNT

\( E = -6616.0992 \text{ Ha} \)

| O2+2O+(6,6)SWCNT cell=[19.2, 19.2, 17.2287] |
|-----------------|-----------------|-----------------|
| O               | 5.628423         | 8.660815        | 0.556500        |
| C               | 5.609262         | 10.071398       | 0.553119        |
| O               | 6.926415         | 12.523235       | 0.572765        |
| C               | 8.109758         | 13.298254       | 0.587385        |
| O               | 10.888281        | 13.552824       | 0.589420        |
| C               | 7.058368         | 6.275294        | 0.621404        |
| O               | 10.161097        | 12.922008       | 0.590748        |
| C               | 13.515473        | 10.510458       | 0.641381        |
| O               | 13.517741        | 9.069277        | 0.658035        |
| C               | 12.303907        | 5.614346        | 0.657894        |
| O               | 12.242219        | 6.616122        | 0.675591        |
| C               | 11.074230        | 5.813328        | 0.677694        |
| O               | 7.782631         | 7.995365        | 1.798882        |
| C               | 7.746967         | 10.774362       | 1.789745        |
| O               | 6.435330         | 12.011419       | 1.801155        |
| C               | 6.515091         | 6.786493        | 1.826401        |
| O               | 8.790735         | 13.500613       | 1.822745        |
| C               | 10.200032        | 13.630028       | 1.835995        |
| O               | 12.702245        | 12.468373       | 1.810947        |
| C               | 13.327916        | 11.227323       | 1.856790        |
| O               | 13.320332        | 8.424311        | 1.896824        |
| C               | 12.678243        | 7.166610        | 1.908275        |
| O               | 8.937780         | 5.493223        | 1.901672        |
| C               | 10.383395        | 5.594852        | 1.913589        |
| O               | 12.644305        | 12.395771       | 16.602873       |
| C               | 6.464564         | 11.995142       | 16.562243       |
| O               | 10.227479        | 5.816583        | 6.857073        |
| C               | 8.823337         | 5.693572        | 6.864017        |
| O               | 6.300680         | 6.762979        | 6.685719        |
| C               | 5.595018         | 7.995285        | 6.693026        |
| O               | 5.749232         | 10.786069       | 6.724817        |
| C               | 6.448630         | 12.017228       | 6.730664        |
| O               | 8.808016         | 13.517096       | 6.740008        |
| C               | 10.212842        | 13.629328       | 6.755556        |
| O               | 13.562697        | 10.536467       | 5.558020        |
| C               | 13.513715        | 9.122798        | 5.572084        |
| O               | 8.767781         | 13.559388       | 16.590001       |
| C               | 12.137684        | 6.704021        | 6.507092        |
| O               | 10.939830        | 5.953201        | 5.626935        |
| C               | 8.180532         | 5.719503        | 5.589592        |
| O               | 6.911241         | 6.323262        | 5.501782        |
| C               | 5.479274         | 8.694775        | 5.481356        |
| O               | 5.526531         | 10.114402       | 5.488917        |
| C               | 6.936893         | 12.521889       | 5.499435        |
| O               | 8.136888         | 13.267637       | 5.506185        |
| C               | 10.929022        | 13.476719       | 5.536953        |
| O               | 12.210793        | 12.937532       | 5.583076        |
| C               | 10.184250        | 13.677244       | 16.602613       |
| O               | 12.966675        | 12.634840       | 4.341499        |
| C               | 13.413632        | 11.220761       | 4.336408        |
| O               | 13.310232        | 8.440756        | 4.352808        |
| C               | 12.642280        | 7.191400        | 4.369436        |
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