

## Supporting Information:

### Isomerization of Surface Functionalized SWCNTs and the Critical Influence on Photoluminescence: Static Calculations and Excited-State Dynamics Simulations

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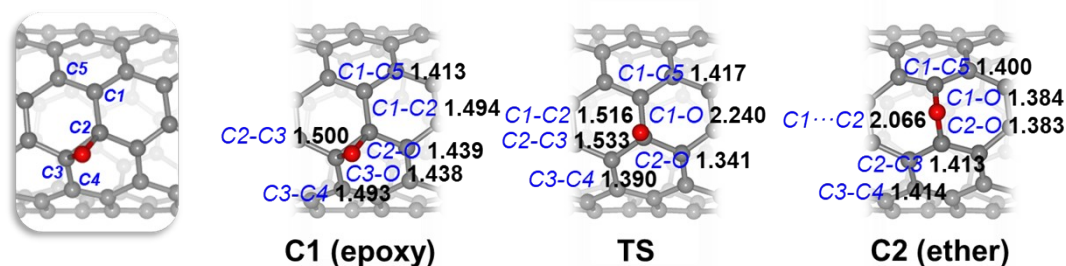


Fig. S1. Structural parameters of the studied reaction path for oxygen functionalized SWCNT fragment (bond lengths in Å).

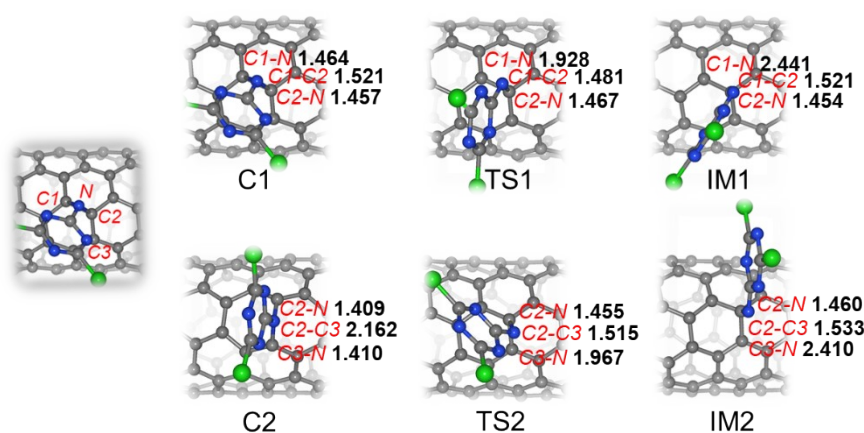


Fig. S2. Key structural parameters of the studied reaction paths for triazine group functionalized SWCNT fragment (bond lengths in Å).

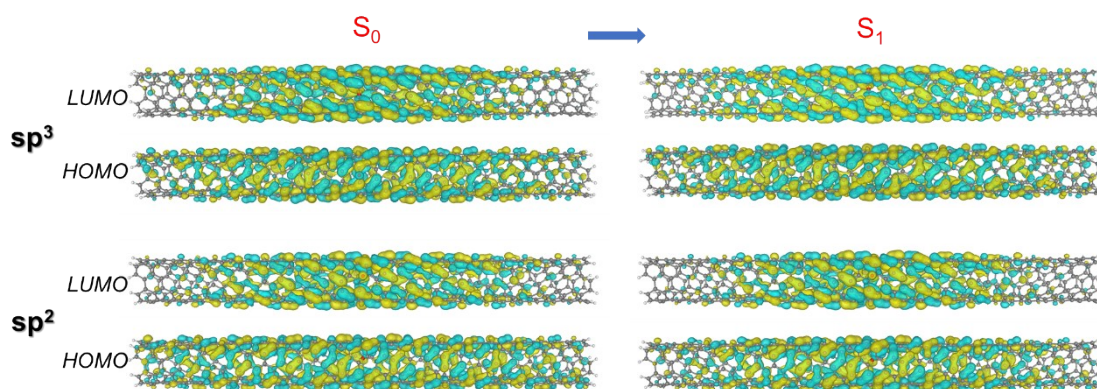


Fig. S3. HOMO-LUMO spatial distributions of oxygen functionalized SWCNT fragment in the relaxed  $S_0$  and  $S_1$  state. The structural model contains 751 atoms with a length of  $\sim 8$  nm.

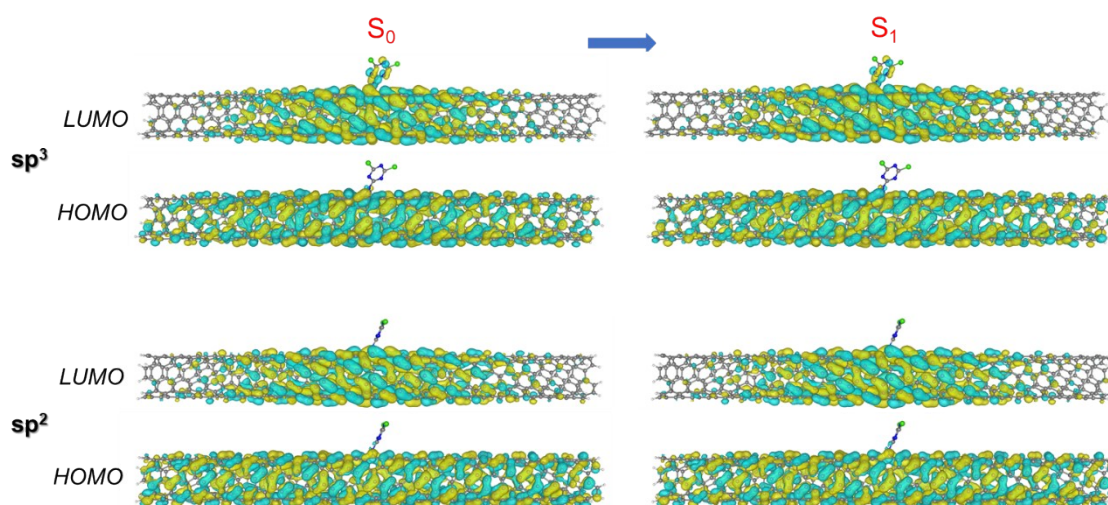


Fig. S4. HOMO-LUMO spatial distributions of triazine group functionalized SWCNT fragment in the relaxed  $S_0$  and  $S_1$  state. The structural model contains 759 atoms with a length of  $\sim 8$  nm.

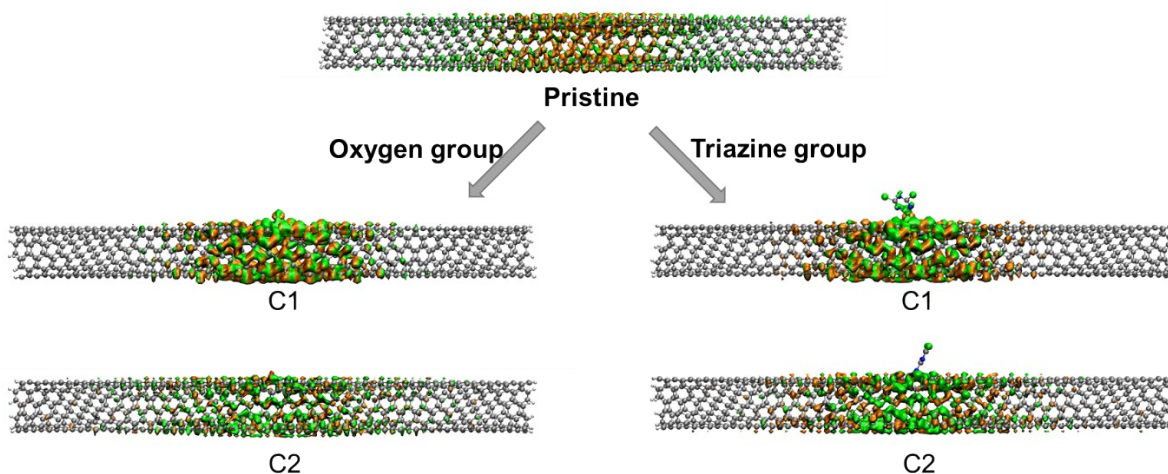


Fig. S5. Electron-hole distribution of the oxygen and triazine group functionalized SWCNT fragments in the relaxed  $S_1$  state. The orange nodes represent the spatial distribution of the photogenerated hole, whereas the green ones denote the electron.

Table S1. Atomic coordinates (XYZ form) of the  $sp^3$  configuration of oxidized SWCNT fragment.

C	-9.08872400	1.91914200	-2.80114400	C	1.30435300	-3.26133600	-1.25055100
C	-8.94625900	2.87847900	-1.84141200	C	1.63258900	1.19068800	3.15537200
C	-9.06663000	-2.05096600	2.80264200	C	1.79409000	-0.18969400	3.39485700
C	-8.91741900	-3.01410500	1.84434300	C	1.63496300	-1.26045500	-3.16937100
C	-8.59046700	3.34283400	1.06663500	C	1.79404200	0.12636600	-3.38618500
C	-8.41727100	2.77134700	2.30612500	C	2.12251200	-2.69854200	2.21653600
C	-8.55966400	-3.48307800	-1.05748000	C	2.28566400	-3.37604000	0.98064900
C	-8.39855600	-2.90205100	-2.29362400	C	2.13735100	2.64098900	-2.21935500
C	-8.08060300	0.11094300	3.49891100	C	2.31679700	3.31404200	-0.97601300
C	-7.94183100	-1.27072100	3.21150800	C	2.61747700	-3.00555700	-1.76258600
C	-8.08838400	-0.23546300	-3.49127200	C	2.77759800	-2.01999200	-2.78834600
C	-7.95669600	1.14172800	-3.20699400	C	2.62645800	2.93493300	1.75824600
C	-7.63744700	-3.27914100	1.26906800	C	2.78068900	1.95147000	2.79109700
C	-7.47043500	-3.55560800	-0.15206300	C	3.09737500	0.69794100	-3.35258300
C	-7.66575400	3.14857600	-1.26267600	C	3.25626400	2.02190200	-2.79334600
C	-7.50418400	3.42224900	0.15959600	C	3.09451600	-0.76521800	3.35553900
C	-7.14062900	-2.39068100	-2.69352800	C	3.25501800	-2.08390900	2.79893000
C	-6.99602900	-1.08509600	-3.36400100	C	3.60402100	3.42149100	-0.41610900
C	-7.15290800	2.27718600	2.70683200	C	3.75597100	3.27903900	0.99858300
C	-6.99879800	0.96690100	3.37663900	C	3.57969300	-3.50185500	0.42461000
C	-6.67522800	1.66737500	-2.93726700	C	3.74070300	-3.36022100	-0.99844600
C	-6.53514100	2.71462300	-1.97074700	C	4.06555300	1.44795600	3.07262800
C	-6.65914500	-1.78482500	2.93918600	C	4.22331700	0.07068300	3.40515300
C	-6.50851900	-2.83363600	1.97686000	C	4.06526100	-1.51706100	-3.06576400
C	-6.21497300	3.32612000	0.71765000	C	4.22230800	-0.13738300	-3.40022800
C	-6.03521300	2.77273100	2.02095900	C	4.54852400	-2.51515400	2.42145800
C	-6.18141200	-3.44605900	-0.70948500	C	4.71017700	-3.27435700	1.24008500
C	-6.01519900	-2.88240600	-2.01195900	C	4.56488100	2.44172500	-2.41203800
C	-5.68427700	0.39743500	3.41449900	C	4.73770900	3.19036500	-1.23600400
C	-5.51888500	-0.99828100	3.27010500	C	5.04455200	-3.11558200	-1.51494500
C	-5.68913200	-0.50469900	-3.40705400	C	5.20650500	-2.22925000	-2.59312800
C	-5.52945800	0.89163600	-3.26378400	C	5.06448100	3.03534600	1.52106400
C	-5.19165500	-3.12595800	1.49235500	C	5.21810900	2.15584600	2.59991300
C	-5.02694200	-3.49426000	0.14213700	C	5.54558700	0.43149900	-3.36757300
C	-5.21938500	3.01201100	-1.48190100	C	5.71859300	1.76639000	-2.93573100
C	-5.06438500	3.38021800	-0.13476400	C	5.53927300	-0.50622000	3.37049500
C	-4.69084300	-2.50645300	-2.43582700	C	5.70554600	-1.84130500	2.93831100
C	-4.53219400	-1.32254900	-3.20682900	C	6.05900100	3.36212700	-0.69260800
C	-4.69688700	2.41603800	2.44407200	C	6.21812000	3.34458200	0.73283500
C	-4.53381500	1.22274800	3.22387700	C	6.03381700	-3.44482600	0.69822900
C	-4.22251400	1.44314100	-3.06715300	C	6.19720900	-3.42623900	-0.72440400
C	-4.07500900	2.57775500	-2.19895600	C	6.52742800	1.69512700	2.93998400
C	-4.21401300	-1.54324300	3.08135300	C	6.67485800	0.33993800	3.39331200
C	-4.05666100	-2.68089400	2.21775700	C	6.52004400	-1.77575200	-2.93065500
C	-3.76920800	3.42508400	0.43048000	C	6.67352600	-0.42047200	-3.38580700

C	-3.59051400	2.95962600	1.79967500	C	7.00939900	-2.34395900	2.65713200
C	-3.72987500	-3.50295200	-0.42478000	C	7.15764300	-3.25949700	1.51581700
C	-3.56699100	-3.03889300	-1.78157200	C	7.02427900	2.25936500	-2.64933200
C	-3.25010400	0.67206500	3.36101700	C	7.18025400	3.16876300	-1.50804500
C	-3.08815800	-0.75217300	3.35590200	C	7.48494900	-3.28726700	-1.27870500
C	-3.24467100	-0.76394500	-3.35726000	C	7.64634300	-2.46794300	-2.46167000
C	-3.09004000	0.66379900	-3.33256500	C	7.50417700	3.19744100	1.28702100
C	-2.76754200	-3.01866000	1.75746200	C	7.66009100	2.37975600	2.46804300
C	-2.60387500	-3.48756600	0.42201200	C	7.96676900	0.15497900	-3.41089700
C	-2.79277300	2.93702200	-1.72963900	C	8.11662000	1.51529100	-3.10762600
C	-2.66292200	3.42405400	-0.41178800	C	7.96174700	-0.24381500	3.42105500
C	-2.26742600	-2.68488200	-2.22669500	C	8.10312500	-1.60786000	3.11656900
C	-2.10525800	-1.55971100	-3.06989800	C	8.45033300	3.45905500	-0.93043000
C	-2.26897900	2.59976800	2.21520300	C	8.60711900	3.48988000	0.42815700
C	-2.10534800	1.47137300	3.05205300	C	8.42316000	-3.55463900	0.93979300
C	-1.78270600	1.21906900	-3.14003600	C	8.58282900	-3.58483900	-0.42110800
C	-1.62088600	2.41297700	-2.39551700	C	8.94668000	1.90583900	2.90279600
C	-1.78004700	-1.30106700	3.18268800	C	9.09342500	0.64331100	3.38427900
C	-1.61996400	-2.48690400	2.42690700	C	8.93675800	-2.00259000	-2.89565000
C	-1.32372900	3.66962200	0.17211200	C	9.09250200	-0.74095400	-3.37563600
C	-1.12974600	3.14320100	1.55569900	H	-10.07953700	1.63680000	-3.14659000
C	-1.28755000	-3.51356400	-0.14607300	H	-9.83289000	3.35508600	-1.43540200
C	-1.12244000	-3.16036700	-1.51363700	H	-10.06070400	-1.77078000	3.14050900
C	-0.80355700	0.94199500	3.26163900	H	-9.80261700	-3.49035700	1.43503700
C	-0.64124600	-0.48097000	3.40118100	H	-9.59912100	3.57104100	0.73818200
C	-0.79689900	-1.02037400	-3.27337900	H	-9.29658000	2.56834800	2.90966600
C	-0.64064100	0.40295100	-3.36547100	H	-9.56456500	-3.72386500	-0.72654000
C	-0.32128200	-2.87586000	2.00684500	H	-9.28214900	-2.70602600	-2.89315500
C	-0.15898600	-3.45907300	0.70067900	H	-9.09075500	0.50824900	3.50910700
C	-0.32603900	2.84610800	-2.03025700	H	-9.09517700	-0.64103500	-3.50568600
C	-0.14290400	3.59412600	-0.74985500	H	9.12666400	1.88491200	-2.96097100
C	0.16972500	-2.86370800	-2.00191900	H	9.11159000	-1.98139000	2.96895000
C	0.32891700	-1.79235000	-2.94517300	H	9.33044400	3.53304300	-1.56168800
C	0.14400900	2.79369900	1.98856000	H	9.60702400	3.58578500	0.83820200
C	0.31916800	1.71533000	2.91421800	H	9.30411200	-3.62475900	1.57038000
C	0.64538700	0.96604600	-3.24330000	H	9.58437200	-3.67754200	-0.82783600
C	0.79765700	2.22532400	-2.58846200	H	9.82697500	2.52159500	2.74792000
C	0.64529000	-1.03838900	3.27553500	H	10.08257600	0.25079300	3.60328100
C	0.80742500	-2.29044500	2.61724400	H	9.81220700	-2.62586700	-2.74322400
C	1.18717500	3.43819600	-0.12734600	H	10.08413400	-0.35533600	-3.59563800
C	1.32218700	3.18593000	1.22462500	O	-0.73690100	4.85043200	-0.39150700
C	1.13908400	-3.51125900	0.13328000				

Table S2. Atomic coordinates (XYZ form) of the transition state for oxygen migration on the surface of the SWCNT fragment.

C	-9.09712200	2.22542100	-2.56163800	C	1.30630800	-3.13786400	-1.56025100
C	-8.95110000	3.08085900	-1.51961600	C	1.64399900	0.87506600	3.25765200
C	-9.10227800	-2.33184400	2.56974300	C	1.79999000	-0.53228000	3.36320000
C	-8.95008800	-3.19182100	1.53179500	C	1.63617600	-0.95945200	-3.26880800
C	-8.60270800	3.22734600	1.41253400	C	1.79479800	0.44754800	-3.33701300
C	-8.44078000	2.52613900	2.57072700	C	2.12013100	-2.91568900	1.94885300
C	-8.58876500	-3.33935400	-1.39761200	C	2.28055300	-3.47579500	0.64590100
C	-8.42674000	-2.63572700	-2.55613800	C	2.12961900	2.84048800	-1.90937300
C	-8.11333800	-0.24743900	3.45136300	C	2.30414200	3.45109000	-0.61726800
C	-7.97178200	-1.57465400	3.04652100	C	2.61128200	-2.83550200	-2.04500700
C	-8.10143000	0.14229900	-3.43548400	C	2.77250300	-1.75002100	-2.96681400
C	-7.96077300	1.47414400	-3.03444500	C	2.62489900	2.75025800	2.04406300
C	-7.65609200	-3.37598300	0.92186100	C	2.77947900	1.65800500	2.96030000
C	-7.48998800	-3.51128900	-0.49691500	C	3.08803100	1.01440700	-3.21912200
C	-7.65904700	3.27012300	-0.90703900	C	3.24287500	2.27869000	-2.53798400
C	-7.49952300	3.40241200	0.51470300	C	3.09335300	-1.10185900	3.25403200
C	-7.15395100	-2.07767700	-2.88730600	C	3.25138700	-2.35285000	2.57790100
C	-7.00124200	-0.72721500	-3.41813400	C	3.59523300	3.46333500	-0.05366000
C	-7.16369300	1.97565000	2.90813000	C	3.75820100	3.17831900	1.33029400
C	-7.01039900	0.62468200	3.43895000	C	3.57481000	-3.53153700	0.07716800
C	-6.67017100	1.96731100	-2.72333300	C	3.73780800	-3.25951200	-1.31176000
C	-6.52237200	2.92891300	-1.66721100	C	4.07661900	1.11896300	3.18146600
C	-6.67654500	-2.06819100	2.74222600	C	4.23354700	-0.26800700	3.38242000
C	-6.52265900	-3.02530000	1.68619300	C	4.06394800	-1.20917300	-3.17171100
C	-6.21002000	3.26014800	1.06289700	C	4.22076800	0.18699800	-3.35895200
C	-6.04107800	2.56133300	2.30681500	C	4.55595300	-2.74721400	2.15554300
C	-6.19630500	-3.36294900	-1.04342600	C	4.71593800	-3.39278800	0.91913700
C	-6.02892200	-2.66420700	-2.28423200	C	4.56283400	2.66165600	-2.12603200
C	-5.71126700	0.05186000	3.44134500	C	4.73699800	3.30345100	-0.89745200
C	-5.54637300	-1.32704100	3.15443600	C	5.04914800	-2.96566300	-1.80361300
C	-5.69933800	-0.15202500	-3.41432500	C	5.21028000	-1.97394700	-2.78419500
C	-5.53371000	1.22470100	-3.12386100	C	5.07227400	2.87530500	1.82243700
C	-5.21609600	-3.26256100	1.17352800	C	5.22900000	1.88372800	2.80183700
C	-5.05143000	-3.49265200	-0.20453900	C	5.54466800	0.75417800	-3.27971300
C	-5.21906300	3.16897800	-1.14855500	C	5.71523200	2.04648100	-2.72261400
C	-5.06443500	3.39208400	0.22437700	C	5.54939400	-0.84368200	3.30205600
C	-4.71174900	-2.23777500	-2.65900200	C	5.71295600	-2.13692500	2.74461400
C	-4.54866100	-0.99316800	-3.30036500	C	6.05686900	3.42685400	-0.34510600
C	-4.72098300	2.13125900	2.67379800	C	6.22132200	3.26459200	1.07488000
C	-4.55751600	0.89273400	3.31270900	C	6.03468000	-3.52092900	0.36387000
C	-4.22111500	1.73899300	-2.85768200	C	6.19765700	-3.35814800	-1.05368200
C	-4.05921400	2.79239400	-1.91065300	C	6.53324200	1.38813900	3.09016000
C	-4.23325400	-1.84098300	2.88987200	C	6.68116600	-0.00645100	3.40083500
C	-4.07363300	-2.87265800	1.93941100	C	6.51753700	-1.48440600	-3.07299400

C	-3.75042200	3.34281000	0.79045600	C	6.66931600	-0.08768500	-3.38578300
C	-3.58110600	2.75022100	2.07605600	C	7.01243200	-2.60681900	2.40849800
C	-3.74161800	-3.42073000	-0.77009300	C	7.15842900	-3.40564000	1.19375800
C	-3.57532700	-2.84699500	-2.05994100	C	7.01819900	2.50640100	-2.38848400
C	-3.25155600	0.32731000	3.40687300	C	7.17543700	3.30279600	-1.17552000
C	-3.09110500	-1.08237900	3.26897500	C	7.48643900	-3.14933300	-1.58820700
C	-3.24813400	-0.42618600	-3.39002800	C	7.64650200	-2.21984700	-2.67364600
C	-3.08813300	0.98403000	-3.22895700	C	7.51077800	3.04604300	1.60400400
C	-2.77243200	-3.17408700	1.45132200	C	7.66854800	2.11698700	2.68552000
C	-2.60862200	-3.51906500	0.07711900	C	7.96678500	0.48873700	-3.34716800
C	-2.77918500	3.10493900	-1.42572600	C	8.11732900	1.80657000	-2.92017300
C	-2.62538100	3.49199900	-0.04079100	C	7.97381700	-0.59232300	3.36305300
C	-2.27422100	-2.46384800	-2.47952600	C	8.11491600	-1.91345300	2.93693400
C	-2.11129200	-1.25558100	-3.21298400	C	8.45442000	3.53459800	-0.57383200
C	-2.28599300	2.36304800	2.46890100	C	8.61710800	3.43183300	0.77502100
C	-2.11872200	1.15364200	3.20594000	C	8.43049800	-3.64304000	0.58820100
C	-1.78720400	1.50879300	-2.98480900	C	8.59005700	-3.53880700	-0.76340100
C	-1.62502700	2.61474700	-2.11489800	C	8.95901100	1.60046500	3.07466700
C	-1.79608500	-1.61220200	3.04722200	C	9.10700500	0.29953700	3.42603000
C	-1.63601400	-2.72221000	2.16980700	C	8.94045500	-1.71196300	-3.06618000
C	-1.32761600	3.46767000	0.51984900	C	9.09439000	-0.41167000	-3.41495300
C	-1.15440000	2.90787700	1.77995400	H	-10.08360200	2.00152900	-2.95769100
C	-1.30524900	-3.48726300	-0.49205900	H	-9.82699400	3.54797100	-1.08151600
C	-1.13863500	-3.00724200	-1.81917300	H	-10.09166100	-2.11005100	2.95982700
C	-0.81628100	0.59683900	3.32028300	H	-9.82339400	-3.66216900	1.09211500
C	-0.65479800	-0.80150200	3.31232200	H	-9.60161100	3.53031700	1.11640800
C	-0.80782500	-0.69291900	-3.34024400	H	-9.31203600	2.28725200	3.17215700
C	-0.64889800	0.71761500	-3.29998100	H	-9.58873500	-3.63967500	-1.10247200
C	-0.33338800	-3.04661100	1.69312900	H	-9.29903700	-2.39416100	-3.15484200
C	-0.16933100	-3.50159400	0.36492500	H	-9.11991900	0.15311800	3.52019100
C	-0.32834300	2.94143600	-1.64573800	H	-9.10854300	-0.25756000	-3.50183000
C	-0.17454600	3.82816400	-0.42338700	H	9.12615300	2.16647000	-2.74495700
C	0.16442000	-2.64412200	-2.26314900	H	9.12168400	-2.27745600	2.75855400
C	0.32814800	-1.50995200	-3.09410200	H	9.32730300	3.68867000	-1.20069900
C	0.16883300	2.53735600	2.22280500	H	9.61513600	3.50085400	1.19459700
C	0.33085100	1.41986700	3.03772800	H	9.30717400	-3.79085800	1.21115100
C	0.64594400	1.26437300	-3.09148400	H	9.58839200	-3.60357100	-1.18282500
C	0.80109600	2.43421300	-2.31034400	H	9.83579100	2.23569000	2.99769100
C	0.65438400	-1.35380100	3.13204200	H	10.09395800	-0.11181000	3.61828100
C	0.81273200	-2.52930600	2.37623400	H	9.81271700	-2.35415500	-2.99581400
C	1.17150900	3.51288300	0.22907000	H	10.08295300	-0.00635000	-3.61196400
C	1.32507000	3.06726100	1.53918500	O	-0.23933500	5.06005800	-0.93685900
C	1.14099800	-3.51210100	-0.20762500				

Table S3. Atomic coordinates (XYZ form) of the sp<sup>2</sup> configuration of oxidized SWCNT fragment.

C	-9.12256700	2.73347700	-2.01459500	C	1.31314800	-2.75781200	-2.14016200
C	-8.96743400	3.36672400	-0.83112600	C	1.64325400	0.14428500	3.36224600
C	-9.11307800	-2.82869800	2.04528000	C	1.80469700	-1.26471700	3.19328800
C	-8.96252600	-3.46118900	0.86134100	C	1.63168000	-0.25594100	-3.32343100
C	-8.59114500	2.90290400	2.06844200	C	1.78717500	1.14254900	-3.11656500
C	-8.42307600	1.96262900	3.03175900	C	2.12604600	-3.30927500	1.33067500
C	-8.60681400	-2.99726800	-2.03802600	C	2.28624300	-3.57589400	-0.06771100
C	-8.44469400	-2.05727700	-3.00152200	C	2.10412400	3.29013700	-1.32230500
C	-8.11698500	-0.94589200	3.30243000	C	2.27565700	3.56554000	0.08288100
C	-7.97787400	-2.15378600	2.64705900	C	2.60737900	-2.34879100	-2.54380600
C	-8.13244000	0.84936500	-3.27470500	C	2.76474300	-1.08559800	-3.19398700
C	-7.99050400	2.05631500	-2.61930800	C	2.61874200	2.21183000	2.52396600
C	-7.66335600	-3.51611700	0.21610100	C	2.77780800	0.96949600	3.19784400
C	-7.49824100	-3.34414300	-1.17849600	C	3.07650600	1.68301300	-2.90477000
C	-7.66596200	3.42337600	-0.19210900	C	3.23536800	2.79019500	-2.02094400
C	-7.49031200	3.24867400	1.20086200	C	3.10035500	-1.78743800	2.95968200
C	-7.16050200	-1.43348900	-3.20710700	C	3.26142900	-2.86759300	2.05268900
C	-7.01444300	-0.01829000	-3.42507100	C	3.57605800	3.41801100	0.64228200
C	-7.14066700	1.33480400	3.22524600	C	3.74735800	2.80880500	1.90787900
C	-6.99792600	-0.08058900	3.44876900	C	3.58368200	-3.49022300	-0.63587900
C	-6.68639500	2.50108600	-2.23608400	C	3.74502600	-2.91545600	-1.91321900
C	-6.53055500	3.24357800	-1.02502600	C	4.08430000	0.40986300	3.31069000
C	-6.67567400	-2.60085800	2.26136400	C	4.24749800	-0.98168300	3.24442700
C	-6.52342900	-3.33735400	1.04266400	C	4.06409600	-0.51094300	-3.29350000
C	-6.18578100	3.00344600	1.70597300	C	4.22046500	0.88258500	-3.20474800
C	-6.01443900	2.04076400	2.75990700	C	4.57560400	-3.16747000	1.55965500
C	-6.19830300	-3.10453900	-1.69521800	C	4.73515500	-3.53821400	0.21913800
C	-6.03292200	-2.14820900	-2.75972400	C	4.55518000	3.08535600	-1.54581500
C	-5.70282700	-0.65482500	3.35026900	C	4.72524100	3.46080000	-0.20993000
C	-5.54551600	-1.96513800	2.80876400	C	5.05913500	-2.52673500	-2.34390800
C	-5.71699800	0.55135000	-3.32657900	C	5.21453900	-1.34459400	-3.09147600
C	-5.55529500	1.85986400	-2.77821100	C	5.06171000	2.42878600	2.33857500
C	-5.22475900	-3.47997800	0.49329000	C	5.22574400	1.24930600	3.09166100
C	-5.06095600	-3.40880200	-0.90612800	C	5.53715000	1.42951700	-3.03954900
C	-5.22901900	3.39834100	-0.48405400	C	5.70537600	2.59708600	-2.24692100
C	-5.05386200	3.32130100	0.91231300	C	5.56275900	-1.52301400	3.05986900
C	-4.72577700	-1.64405000	-3.02011900	C	5.72963100	-2.68736800	2.25803900
C	-4.56799100	-0.29460600	-3.36065900	C	6.03881400	3.46015400	0.35731100
C	-4.70440400	1.53067600	3.00148100	C	6.20503900	2.98095800	1.70300800
C	-4.54846800	0.18497500	3.36628100	C	6.04526200	-3.54400400	-0.35433500
C	-4.24840100	2.31855600	-2.41781000	C	6.20486900	-3.06947600	-1.70482700
C	-4.08287800	3.16197000	-1.30829900	C	6.52906200	0.71624300	3.27217900
C	-4.23651800	-2.42800700	2.45030100	C	6.68682800	-0.70845100	3.30296800
C	-4.07706100	-3.23905000	1.31964300	C	6.51329500	-0.80330000	-3.27382200
C	-3.72847400	3.12331900	1.42524500	C	6.66341700	0.62287700	-3.29960300

C	-3.56008000	2.24209500	2.50716400	C	7.02756800	-3.06020900	1.82130700
C	-3.74107700	-3.21201400	-1.43967300	C	7.17378000	-3.58573600	0.48032900
C	-3.57470600	-2.36202200	-2.54301800	C	7.00607300	2.97817300	-1.82374200
C	-3.23986200	-0.40338000	3.35673000	C	7.16143400	3.50645600	-0.48358300
C	-3.08335000	-1.75152800	2.96402500	C	7.49727900	-2.73619800	-2.17615500
C	-3.25499700	0.28460300	-3.33292100	C	7.65292300	-1.60460200	-3.02511700
C	-3.10040500	1.61561800	-2.91158500	C	7.50079300	2.65399600	2.17004200
C	-2.76548200	-3.45715400	0.78624400	C	7.66437600	1.52291600	3.01799600
C	-2.60163600	-3.50066000	-0.62828800	C	7.96416500	1.18581200	-3.15209200
C	-2.76757300	3.44007500	-0.79440300	C	8.11258400	2.39074800	-2.48233100
C	-2.59257300	3.47140800	0.61880900	C	7.98981500	-1.26582600	3.14385200
C	-2.27053900	-1.90351300	-2.88348000	C	8.13830400	-2.46923300	2.47341300
C	-2.10983200	-0.55772600	-3.33848900	C	8.44339600	3.62001000	0.15651800
C	-2.25867800	1.76337100	2.83085200	C	8.60631500	3.22893400	1.44800300
C	-2.10077400	0.43798200	3.32503400	C	8.45336100	-3.69694500	-0.16672200
C	-1.80861300	2.12139500	-2.62786300	C	8.60890900	-3.30637200	-1.45861100
C	-1.65915400	3.17211300	-1.67596800	C	8.96172500	0.94849400	3.30630000
C	-1.78877400	-2.24781800	2.66390800	C	9.11816100	-0.39251100	3.39147900
C	-1.63212000	-3.16958000	1.58145700	C	8.94629700	-1.02379800	-3.31863700
C	-1.29420800	3.35228000	1.23795500	C	9.09527000	0.31795100	-3.40567300
C	-1.13099200	2.43803200	2.32117100	H	-10.10835800	2.61048300	-2.45418200
C	-1.30578400	-3.34998600	-1.17607500	H	-9.83479500	3.76622200	-0.31500900
C	-1.14130800	-2.57148100	-2.35810100	H	-10.09696000	-2.70615700	2.48925800
C	-0.80391100	-0.13662700	3.36137300	H	-9.83146700	-3.86192000	0.34892500
C	-0.64726500	-1.51457500	3.08204700	H	-9.58330900	3.29448900	1.86959100
C	-0.81935500	0.02068800	-3.34793300	H	-9.28291000	1.61846700	3.59802900
C	-0.66132400	1.40113700	-3.03898500	H	-9.59752600	-3.38907600	-1.83273800
C	-0.32693300	-3.39015400	1.05080700	H	-9.30779200	-1.71176300	-3.56195800
C	-0.16344800	-3.53629600	-0.33872500	H	-9.12031800	-0.56260600	3.45840900
C	-0.36987100	3.62350100	-1.39057600	H	-9.13642300	0.46795300	-3.43095300
C	-0.13422500	3.83325800	0.61887000	H	9.11987800	2.71845000	-2.24542700
C	0.16632100	-2.11615900	-2.70851900	H	9.14502900	-2.79384400	2.23005700
C	0.32615400	-0.82932100	-3.25081200	H	9.31075600	3.92455000	-0.42099100
C	0.17641000	1.99638400	2.68881600	H	9.60089600	3.22384300	1.88132300
C	0.34013800	0.71344900	3.26117900	H	9.32384000	-4.00061300	0.40652400
C	0.64599600	1.91074900	-2.75773000	H	9.60094900	-3.29957900	-1.89772300
C	0.80388900	3.02028500	-1.89491200	H	9.83047600	1.59594900	3.37055100
C	0.66458300	-2.02620100	2.81205800	H	10.10570900	-0.82830900	3.51443900
C	0.82521900	-3.02502300	1.82850700	H	9.81817300	-1.66665200	-3.38665200
C	1.16904400	3.45743800	0.99481900	H	10.07998200	0.75863800	-3.53385200
C	1.32575600	2.63448200	2.13730500	O	-0.25005700	4.65914400	-0.48242700
C	1.15084900	-3.43187300	-0.90356300				