Supporting Information

An Investigation of Electrocatalytic Activity of the FeCe Nanoparticle Encapsulated Carbon Nanotube towards Oxygen Reduction Reaction

Dikeshwar Halba[1], Lokesh Yadav[1] and Srimanta Pakhira[1,2*]

1 Theoretical Condensed Matter Physics and Advanced Computational Materials Science Laboratory, Department of Physics, Indian Institute of Technology Indore (IIT Indore), Simrol, Khandwa Road, Indore-453552, Madhya Pradesh, India.

2 Theoretical Condensed Matter Physics and Advanced Computational Materials Science Laboratory, Centre for Advanced Electronics (CAE), Indian Institute of Technology Indore, Simrol, Khandwa Road, Indore-453552, Madhya Pradesh, India.

*Corresponding author: spakhira@iiti.ac.in (or) spakhirafsu@gmail.com

.CIF format of all the equilibrium structures involved in the associative mechanism of ORR on the surface of FeCe@CNT material is provided below.

1. Equilibrium FeCe@CNT (.cif format)

```
_chemical_name_common                  ' FeCe@CNT '
_cell_length_a                         21.652761
_cell_length_b                         21.652761
_cell_length_c                         2.492334
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      120.000000
_cell_volume                           1011.960212
_space_group_name_H-M_alt              ' P 1 '
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   C001      1.0    0.213649     0.099968     0.000000
   C002      1.0   -0.099968     0.113681     0.000000
   C003      1.0   -0.113681    -0.213649     0.000000
```

C004	1.0	0.180324	0.210584	0.000000
C005	1.0	-0.210584	-0.030259	0.000000
C006	1.0	0.030259	-0.180324	0.000000
C007	1.0	-0.225698	-0.103393	0.000000
C008	1.0	0.103393	-0.122305	0.000000
C009	1.0	0.122305	0.225698	0.000000
C010	1.0	-0.167970	-0.194681	0.000000
C011	1.0	0.194681	0.026711	0.000000
C012	1.0	-0.026711	0.167970	0.000000
C013	1.0	0.215084	0.133556	-0.500000
C014	1.0	-0.133556	0.081528	-0.500000
C015	1.0	-0.081528	-0.215084	-0.500000
C016	1.0	0.200008	0.191807	-0.500000
C017	1.0	-0.191807	0.008201	-0.500000
C018	1.0	-0.008201	-0.200008	-0.500000
FE019	1.0	0.079456	0.091218	-0.500000
FE020	1.0	-0.091218	-0.011762	-0.500000
FE021	1.0	0.011762	-0.079456	-0.500000
C022	1.0	-0.220177	-0.133249	-0.500000
C023	1.0	0.133249	-0.086928	-0.500000
C024	1.0	0.086928	0.220177	-0.500000
C025	1.0	-0.189190	-0.178344	-0.500000
C026	1.0	0.178344	-0.010846	-0.500000
C027	1.0	0.010846	0.189190	-0.500000
CE028	1.0	0.000000	0.000000	0.000000

2. Equilibrium O_2_FeCe@CNT (.cif format)

_chemical_name_common	' O_2_FeCe@CNT '
_cell_length_a	21.587086
_cell_length_b	21.587086

```
_cell_length_c                      2.509098
_cell_angle_alpha                   90.000000
_cell_angle_beta                    90.000000
_cell_angle_gamma                   120.000000
_cell_volume                        1012.596210
_space_group_name_H-M_alt           ' P 1 '
_space_group_IT_number              1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  C001      1.0    0.214599    0.097164    0.000000
  C002      1.0   -0.097164    0.117436    0.000000
  C003      1.0   -0.117436   -0.214599    0.000000
  C004      1.0    0.185610    0.211124    0.000000
  C005      1.0   -0.211124   -0.025513    0.000000
  C006      1.0    0.025513   -0.185610    0.000000
  C007      1.0   -0.225404   -0.098568    0.000000
  C008      1.0    0.098568   -0.126837    0.000000
  C009      1.0    0.126837    0.225404    0.000000
```

C010	1.0	-0.169978	-0.192963	0.000000
C011	1.0	0.192963	0.022985	0.000000
C012	1.0	-0.022985	0.169978	0.000000
C013	1.0	0.217652	0.131710	-0.500000
C014	1.0	-0.131710	0.085941	-0.500000
C015	1.0	-0.085941	-0.217652	-0.500000
C016	1.0	0.204219	0.190975	-0.500000
C017	1.0	-0.190975	0.013244	-0.500000
C018	1.0	-0.013244	-0.204219	-0.500000
FE019	1.0	0.082220	0.093278	-0.500000
FE020	1.0	-0.093278	-0.011058	-0.500000
FE021	1.0	0.011058	-0.082220	-0.500000
C022	1.0	-0.220210	-0.129060	-0.500000
C023	1.0	0.129060	-0.091151	-0.500000
C024	1.0	0.091151	0.220210	-0.500000
C025	1.0	-0.190295	-0.175380	-0.500000
C026	1.0	0.175380	-0.014915	-0.500000
C027	1.0	0.014915	0.190295	-0.500000
CE028	1.0	0.000000	0.000000	0.000000
O029	1.0	0.357136	0.258625	-0.500000
O030	1.0	-0.258625	0.098511	-0.500000
O031	1.0	-0.098511	-0.357136	-0.500000
O032	1.0	0.395003	0.326883	-0.500000
O033	1.0	-0.326883	0.068120	-0.500000
O034	1.0	-0.068120	-0.395003	-0.500000

3. Equilibrium OOH_FeCe@CNT (.cif format)

```
_chemical_name_common                  ' OOH_FeCe@CNT '
_cell_length_a                         21.845076
_cell_length_b                         21.845076
```

```
_cell_length_c                         3.500000
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      120.000000
_cell_volume                           1446.457842
_space_group_name_H-M_alt              ' P 1 '
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  C001      1.0    0.204737    0.095489    0.000000
  C002      1.0   -0.095489    0.109248    0.000000
  C003      1.0   -0.109248   -0.204737    0.000000
  C004      1.0    0.190276    0.208311    0.000000
  C005      1.0   -0.208311   -0.018035    0.000000
  C006      1.0    0.018035   -0.190276    0.000000
  C007      1.0   -0.211490   -0.085710    0.000000
  C008      1.0    0.085710   -0.125780    0.000000
  C009      1.0    0.125780    0.211490    0.000000
```

C010	1.0	-0.157414	-0.179063	0.000000
C011	1.0	0.179063	0.021649	0.000000
C012	1.0	-0.021649	0.157414	0.000000
C013	1.0	0.236028	0.139337	0.500000
C014	1.0	-0.139337	0.096691	0.500000
C015	1.0	-0.096691	-0.236028	0.500000
C016	1.0	0.213438	0.195012	0.500000
C017	1.0	-0.195012	0.018426	0.500000
C018	1.0	-0.018426	-0.213438	0.500000
FE019	1.0	0.110687	0.104812	0.500000
FE020	1.0	-0.104812	0.005875	0.500000
FE021	1.0	-0.005875	-0.110687	0.500000
C022	1.0	-0.203836	-0.113995	0.500000
C023	1.0	0.113995	-0.089841	0.500000
C024	1.0	0.089841	0.203836	0.500000
C025	1.0	-0.177233	-0.161495	0.500000
C026	1.0	0.161495	-0.015738	0.500000
C027	1.0	0.015738	0.177233	0.500000
CE028	1.0	-0.000000	-0.000000	0.00000e
O029	1.0	0.311797	0.165546	0.500000
O030	1.0	-0.165546	0.146250	0.500000
O031	1.0	-0.146250	-0.311797	0.500000
O032	1.0	0.349063	0.245175	0.500000
O033	1.0	-0.245175	0.103888	0.500000
O034	1.0	-0.103888	-0.349063	0.500000
H035	1.0	0.396756	0.253171	0.500000
H036	1.0	-0.253171	0.143584	0.500000
H037	1.0	-0.143584	-0.396756	0.500000

4. Equilibrium O_FeCe@CNT (.cif format)

```
_chemical_name_common                  ' O_FeCe@CNT '
_cell_length_a                         22.843216
_cell_length_b                         22.843216
_cell_length_c                         2.476396
_cell_angle_alpha                      90.000000
_cell_angle_beta                       90.000000
_cell_angle_gamma                      120.000000
_cell_volume                           1119.090556
_space_group_name_H-M_alt              ' P 1 '
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   C001       1.0     0.194483     0.110160     0.000000
   C002       1.0    -0.110160     0.084323     0.000000
   C003       1.0    -0.084323    -0.194483     0.000000
   C004       1.0     0.166556     0.209823     0.000000
   C005       1.0    -0.209823    -0.043267     0.000000
   C006       1.0     0.043267    -0.166556     0.000000
```

C007	1.0	-0.204752	-0.103716	0.000000
C008	1.0	0.103716	-0.101037	0.000000
C009	1.0	0.101037	0.204752	0.000000
C010	1.0	-0.136190	-0.177882	0.000000
C011	1.0	0.177882	0.041691	0.000000
C012	1.0	-0.041691	0.136190	0.000000
C013	1.0	0.224252	0.154473	-0.500000
C014	1.0	-0.154473	0.069779	-0.500000
C015	1.0	-0.069779	-0.224252	-0.500000
C016	1.0	0.191409	0.199887	-0.500000
C017	1.0	-0.199887	-0.008478	-0.500000
C018	1.0	0.008478	-0.191409	-0.500000
FE019	1.0	0.100422	0.108072	-0.500000
FE020	1.0	-0.108072	-0.007649	-0.500000
FE021	1.0	0.007649	-0.100422	-0.500000
C022	1.0	-0.193088	-0.127773	-0.500000
C023	1.0	0.127773	-0.065315	-0.500000
C024	1.0	0.065315	0.193088	-0.500000
C025	1.0	-0.159004	-0.165283	-0.500000
C026	1.0	0.165283	0.006279	-0.500000
C027	1.0	-0.006279	0.159004	-0.500000
CE028	1.0	-0.000000	-0.000000	0.000000
O029	1.0	0.292058	0.182795	-0.500000
O030	1.0	-0.182795	0.109263	-0.500000
O031	1.0	-0.109263	-0.292058	-0.500000

5. Equilibrium OH_FeCe@CNT (.cif format)

_chemical_name_common	' OH_FeCe@CNT '
_cell_length_a	18.775288
_cell_length_b	18.775288

```
_cell_length_c                      3.535393
_cell_angle_alpha                   90.000000
_cell_angle_beta                    90.000000
_cell_angle_gamma                   120.000000
_cell_volume                        1079.298385
_space_group_name_H-M_alt           ' P 1 '
_space_group_IT_number              1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  C001      1.0    0.228918    0.084244    0.000000
  C002      1.0   -0.084244    0.144674    0.000000
  C003      1.0   -0.144674   -0.228918    0.000000
  C004      1.0    0.240084    0.238428    0.000000
  C005      1.0   -0.238428    0.001656    0.000000
  C006      1.0   -0.001656   -0.240084    0.000000
  C007      1.0   -0.249878   -0.076909    0.000000
  C008      1.0    0.076909   -0.172970    0.000000
  C009      1.0    0.172970    0.249878    0.000000
```

C010	1.0	-0.198365	-0.196136	0.000000
C011	1.0	0.196136	-0.002230	0.000000
C012	1.0	0.002230	0.198365	0.000000
C013	1.0	0.240347	0.126033	-0.500000
C014	1.0	-0.126033	0.114314	-0.500000
C015	1.0	-0.114314	-0.240347	-0.500000
C016	1.0	0.271882	0.219224	-0.500000
C017	1.0	-0.219224	0.052657	-0.500000
C018	1.0	-0.052657	-0.271882	-0.500000
FE019	1.0	0.098403	0.101442	-0.500000
FE020	1.0	-0.101442	-0.003039	-0.500000
FE021	1.0	0.003039	-0.098403	-0.500000
C022	1.0	-0.246017	-0.114551	-0.500000
C023	1.0	0.114551	-0.131466	-0.500000
C024	1.0	0.131466	0.246017	-0.500000
C025	1.0	-0.217682	-0.172003	-0.500000
C026	1.0	0.172003	-0.045679	-0.500000
C027	1.0	0.045679	0.217682	-0.500000
CE028	1.0	0.000000	0.000000	0.000000
O029	1.0	0.360517	0.266881	-0.500000
O030	1.0	-0.266881	0.093636	-0.500000
O031	1.0	-0.093636	-0.360517	-0.500000
H032	1.0	0.382076	0.229923	-0.500000
H033	1.0	-0.229923	0.152153	-0.500000
H034	1.0	-0.152153	-0.382076	-0.500000