REFERENCE

Angelikopoulos, P. and Bock, H. (2008) Directed self-assembly of surfactants in carbon nanotube materials. Journal of Physical Chemistry B 112(44): 13793-13801.

Angelikopoulos, P., Gromoy, A., Leen, A., Nerushev, O., Bock, H., and Campbell, E. E. B. (2010) Dispersing Individual Single-Wall Carbon Nanotubes in Aqueous Surfactant Solutions Below the CMC. Journal of Physical Chemistry C 114(1): 2-9.

Bao, Q.L., Zhang, H., Yang, J.X., Wang, S., Tong, D.Y., Jose, R., Ramakrishna, S., Lim, C.T., and Loh, K.P. (2010) Graphene-polymer nanofiber membrane for ultrafast photonics. Advanced Functional Materials 20(5): 782-791.

Bonaccorso, F., Sun, Z., Hasan, T., and Ferrari, A.C. (2010) Graphene photonics and optoelectronics. Nature Photonics 4(9): 611-622.

Bruce, C.D., Berkowitz, M.L., Perera, L., and Forbes, M.D.E. (2002) Molecular dynamics simulation of sodium dodecyl sulfate micelle in water: micellar structural characteristics and counterion distribution. Journal of Physical Chemistry B 106(15): 3788-3793.

Cabane, B., Duplessix, R., and Zemb, T. (1985) High-resolution neutron-scattering on ionic surfactant micelles - sds in water. Journal De Physique 46(12): 2161-2178.

Calvaresi, M., Dallavalle, M., and Zerbetto, F. (2009) wrapping nanotubles with micelles, hemimicelles, and cylindrical micelles. Small 5(19): 2191-2198.

Deng, M.G., Li, X.J., Liang, H.J., Caswell, B., and Karniadakis, G.E. (2012) Simulation and modelling of slip flow over surfaces grafted with polymer brushes and glycocalyx fibres. Journal of Fluid Mechanics 711: 192-211.

Dong, X.C., Huang, W., and Chen, P. (2011). In situ synthesis of reduced graphene oxide and gold nanocomposites for nanoelectronics and biosensing. Nanoscale Research Letters 6: 60-65.

Green, A.A. and Hersam, M.C. (2010) Emerging methods for producing monodisperse graphene dispersions. Journal of Physical Chemistry Letters 1(2): 544-549.

Groot, R.D. (2000) Mesoscopic simulation of polymer-surfactant aggregation. langmuir 16(19): 7493-7502.

Groot, R.D. and Rabone, K.L. (2001) Mesoscopic simulation of cell membrane damage, morphology change and rupture by nonionic surfactants. Biophysical Journal 81(2): 725-736.

Groot, R.D. and Warren, P.B. (1997) Dissipative particle dynamics: bridging the gap between atomistic and mesoscopic simulation. Journal of Chemical Physics 107(11): 4423-4435.

Hamilton, C.E., Lomeda, J.R., Sun, Z.Z., Tour, J.M., and Barron, A.R. (2009) High-yield organic dispersions of unfunctionalized graphene. Nano Letters 9(10): 3460-3462.

Han, T.H., Lee, W.J., Lee, D.H., Kim, J.E., Choi, E.Y., and Kim, S.O. (2010) Peptide/graphene hybrid assembly into core/shell nanowires. Advanced Materials 22(18): 2060-2064.

Hu, X., Yu, Y., Hou, W., Zhou, J., and Song, L. (2013) Effects of particle size and ph value on the hydrophilicity of graphene oxide. Applied Surface Science 273: 118-121.

Huang, X.H., Zhou, R.H., and Berne, B.J. (2005) Drying and hydrophobic collapse of paraffin plates. Journal of Physical Chemistry B 109(8): 3546-3552.

Islam, M.F., Rojas, E., Bergey, D.M., Johnson, A.T., and Yodh, A.G. (2003) High weight fraction surfactant solubilization of single-wall carbon nanotubes in water. Nano Letters 3(2): 269-273.

Jalili, S. and Akhavan, M. (2009) A coarse-grained molecular dynamics simulation of a sodium dodecyl sulfate micelle in aqueous solution. Colloids and Surfaces a-Physicochemical and Engineering Aspects 352(1-3): 99-102.

Koelman, J. and Hoogerbrugge, P.J. (1993). Dynamic simulations of hard-sphere suspensions under steady shear. Europhysics Letters 21(3): 363-368.

Konatham, D. and Striolo, A. (2008) Molecular design of stable graphene nanosheets dispersions. Nano Letters 8(12): 4630-4641.

Kuo, M.Y., Yang, H.C., Hua, C.Y., Chen, C.L., Mao, S.Z., Deng, F., Wang, H.H., and Du, Y.R. (2004) Computer simulation of ionic and nonionic mixed surfactants in aqueous solution. Chemphyschem 5(4): 575-580.

Lee, H. and Kim, H. (2012). Self-assembly of lipids and single-walled carbon nanotubes: effects of lipid structure and pegylation. Journal of Physical Chemistry C 116(16): 9327-9333.

Lee, J.H., Shin, D.W., Makotchenko, V.G., Nazarov, A.S., Fedorov, V.E., Yoo, J.H., Yu, S.M., Choi, J.Y., Kim, J.M., and Yoo, J.B. (2010). The superior dispersion of easily soluble graphite. Small 6(1): 58-62.

Liu, N., Luo, F., Wu, H.X., Liu, Y.H., Zhang, C., and Chen, J. (2008) One-step ionic-liquid-assisted electrochemical synthesis of ionic-liquid-functionalized graphene sheets directly from graphite. Advanced Functional Materials 18(10): 1518-1525.

Lu, J.R., Li, Z.X., Thomas, R.K., Staples, E.J., Tucker, I., and Penfold, J. (1993) Neutron reflection from a layer of monododecyl hexaethylene glycol adsorbed at the air-liquid interface: the configuration of the ethylene glycol chain. The Journal of Physical Chemistry 97(30): 8012-8020.

Mackerell, A.D. (1995) Molecular-dynamics simulation analysis of a sodium dodecyl-sulfate micelle in aqueous-solution - decreased fluidity of the micelle hydrocarbon interior. Journal of Physical Chemistry 99(7): 1846-1855.

Min, S.H., Lee, C., and Jang, J. (2012) Dissipative particle dynamics modeling of a graphene nanosheet and its self-assembly with surfactant molecules. Soft Matter 8(33): 8735-8742.

Nagarajan, R. and Wang, C.C. (2000) Theory of surfactant aggregation in water/ethylene glycol mixed solvents. Langmuir 16(12): 5242-5251.

Park, J.H. and Aluru, N.R. (2011) Self-assembly of graphenes. Surface Science 605(17-18): 1616-1620.

Partington, J.R., Hudson, R.F., and Bagnall, K.W. (1952). Self-diffusion of aliphatic alcohols. Nature 169(4301): 583-584.

Rao, C.N.R., Biswas, K., Subrahmanyam, K.S., and Govindaraj, A. (2009). Graphene, the new nanocarbon. Journal of Materials Chemistry 19(17): 2457-2469.

Rekvig, L., Kranenburg, M., Vreede, J., Hafskjold, B., and Smit, B. (2003). Investigation of surfactant efficiency using dissipative particle dynamics. Langmuir 19(20): 8195-8205.

Schweighofer, K.J., Essmann, U., and Berkowitz, M. (1997) Simulation of sodium dodecyl sulfate at the water-vapor and water-carbon tetrachloride interfaces at low surface coverage. Journal of Physical Chemistry B 101(19): 3793-3799.

Shelley, J., Watanabe, K., and Klein, M. L. (1990) Simulation of a sodium dodecyl-sulfate micelle in aqueous-solution. International Journal of Quantum Chemistry: 103-117.

Shih, C.J., Lin, S.C., Sharma, R., Strano, M.S., and Blankschtein, D. (2012). Understanding the ph-dependent behavior of graphene oxide aqueous solutions: a comparative experimental and molecular dynamics simulation study. Langmuir 28(1): 235-241.

Shih, C.J., Lin, S.C., Strano, M.S., and Blankschtein, D. (2010) Understanding the stabilization of liquid-phase-exfoliated graphene in polar solvents: molecular dynamics simulations and kinetic theory of colloid aggregation. Journal of the American Chemical Society 132(41): 14638-14648.

Shin, K.Y., Hong, J.Y., and Jang, J. (2011) Flexible and transparent graphene films as acoustic actuator electrodes using inkjet printing. Chemical Communications 47(30): 8527-8529.

Smith, R.J., Lotya, M. and Coleman, J.N. (2010) The importance of repulsive potential barriers for the dispersion of graphene using surfactants. New Journal of Physics 12(12): 1-10.

Subrahmanyam, K.S., Ghosh, A., Gomathi, A., Govindaraj, A., and Rao, C.N.R. (2009) Covalent and noncovalent functionalization and solubilization of graphene. Nanoscience and Nanotechnology Letters 1(1): 28-31.

Takahash.Y, Sumita, I., and Tadokoro, H. (1973) Structural studies of polyethers .9. planar zigzag modification of poly(ethylene oxide). Journal of Polymer Science Part B-Polymer Physics 11(11): 2113-2122.

Tanford, C. (1972) Micelle shape and size. Journal of Physical Chemistry 76(21): 3020-3024.

Tummala, N.R., Grady, B.P., and Striolo, A. (2010) lateral confinement effects on the structural properties of surfactant aggregates: sds on graphene. Physical Chemistry Chemical Physics 12(40): 13137-13143.

Tummala, N.R., Morrow, B.H., Resasco, D.E. and Striolo, A. (2010). Stabilization of aqueous carbon nanotube dispersions using surfactants: insights from molecular dynamics simulations. Acs Nano 4(12): 7193-7204.

Wilson, M.R. (1996) Determination of order parameters in realistic atom-based models of liquid crystal systems. Journal of Molecular Liquids 68(1): 23-31.

Wu, D. and Yang, X. N. (2012) Coarse-grained molecular simulation of self-assembly for nonionic surfactants on graphene nanostructures. Journal of Physical Chemistry B 116(39): 12048-12056.

Xu, C., Wang, X., and Zhu, J. W. (2008) Graphene-metal particle nanocomposites. Journal of Physical Chemistry C 112(50): 19841-19845.

Zhang, W., Dubois, M., Guerin, K., Bonnet, P., Kharbache, H., Masin, F., Kharitonov, A. P., and Hamwi, A. (2010) Effect of curvature on c-f bonding in fluorinated carbons: from fullerene and derivatives to graphite. Physical Chemistry Chemical Physics 12(6): 1388-1398.

APPENDICES

Appendix A: Visual Fortran code used to calculate the angle distribution of SDS on nanosheets' surfaces and the angles used for order parameter calculation

```
PROGRAM ANGCOUNT

IMPLICIT NONE

INTEGER ii, aa,bb,  im, f, u, t, s, RR , d,e,j, p, ik, ika, k,
n_atom, n_molecule, m, ID_atom , n_frame, N, N_bin, ig, q,a,
ID_mole, L, i, D_ATOM_1, D_ATOM_2 ,D_ATOM_3, skip, ID_type ,
ID_type1,ID_type2, Mole_ID, ix,iy,iz,gap,c

REAL R, Xw, Yw, Zw,Xb,Yb,Zb, Xt, Yt, Zt, BIN_SIZE, Box, Dist,
nidinbin, V_1, RHO, Nid, XRR,YRR,ZRR,XR,YR,ZR,xu, yu,
zu,vxt,vyt,vzt,Box_Lx,Box_Hx, Box_Ly,Box_Hy,Box_Lz,Box_Hz

REAL RNT,XNT, YNT, ZNT , deldeg, RADIAN, THETA, XNTR, YNTR,ZNTR,
ANGLE_TEST,ANGLE,dot,magnitude

INTEGER, ALLOCATABLE::      il(:)

REAL, ALLOCATABLE::                 XA(:), YA(:), ZA(:), X(:) , Y(:)
, Z(:)      , Avgl(:)


REAL, ALLOCATABLE::                 G(:) ,Avg_1(:) , Avg_2(:),
vgh(:)

n_frame  = 1001
n_atom   = 1728
n_molecule = n_atom/3
N_bin    = 180
BIN_SIZE = 180/N_bin
Skip     = 0
Box=((25.1852832-0)+(25.1852832-0)+(25.1852832-0))/3


ALLOCATE( X(1:(n_atom)) , Y(1:(n_atom)) , Z(1:(n_atom)) )

   DO c = 1, n_atom

        X(c)=0; Y(c)=0; Z(c)=0

   END DO

 ALLOCATE( il(1:n_molecule)  )

   DO u = 1, n_molecule

         il(u) = 0
```

```
   END DO
ALLOCATE( G(0:N_bin), Avg_1(0:N_bin) , Avg_2(0:N_bin),vgh(0:N_bin))
   DO a=0,N_bin
         G(a)=0
         Avg_1(a)=0
       Avg_2(a)=0
       vgh(a)=0
   END DO

OPEN(unit=1, file='XIII-23-1001F.xyz', status='old')
OPEN(unit=3, file='FILTERED_BEADS-XIII-23-1001F-X.data',
status='unknown')
OPEN(unit=4, file='ANGLECOUNT-XIII-23-1001F-X.data',
status='unknown')
OPEN(unit=5, file='HOWMANY-XIII.data', status='unknown')
OPEN(unit=6, file='CHECK1-XIII.data', status='unknown')
OPEN(unit=7, file='CHECK2-XIII.data', status='unknown')
OPEN(unit=8, file='ORIENT-XIII.data', status='unknown')
Do i =1, skip
   DO k =1, n_atom + 2
      READ (1,*)
   END DO
END DO

DO i=1,n_frame - skip
   IF ( (i.EQ.1) .OR. (MOD(i,1).EQ.0) ) THEN
         WRITE(*,*) 'frame', i
   END IF

        ik=0

               READ (1,*)
```

```
            READ (1,*)

         DO k=1,n_atom

            READ(1,*)ID_type,Xt, Yt, Zt

              IF ((Xt .GE. 0) .AND. (Xt .LE. 27.72) .AND. (Yt .GE.
0) .AND. (Yt .LE. 27.72) .AND. (Zt .GE. 0) .AND. (Zt .LE. 27.72))
then

              ik=ik+1

                   X(ik)=Xt    ;      Y(ik)=Yt     ;      Z(ik)=Zt

                  END IF


           END DO


           L=ik

           im = 0

           ika = 0


           DO e= 0, L-3, 3

           XR=X(e+3)-X(e+1) ; ZR=Z(e+3)-Z(e+1) ; YR=Y(e+3)-Y(e+1)

           WRITE (6,*) XR, YR, ZR

           IF (Z(e+3) .GE. 13.86) then
           dot = ZR * 1

           magnitude = sqrt((XR*XR)+(YR*YR)+(ZR*ZR))

           ANGLE_TEST = 90-((acos(dot/magnitude))*57.2957795)


           else if (Z(e+3) .LE. 13.86)  then

           dot = ZR * -1

           magnitude = sqrt((XR*XR)+(YR*YR)+(ZR*ZR))

           ANGLE_TEST = 90-((acos(dot/magnitude))*57.2957795)

           END IF

           IF (ANGLE_TEST .LT. 0) then

                  ANGLE_TEST = abs(ANGLE_TEST)
```

```
            end if
            WRITE (7,*) dot, magnitude,ANGLE_TEST

            ig=NINT(ANGLE_TEST/BIN_SIZE)
            G(ig) = G(ig)+1

            END DO
 END DO

         DO i=0, N_bin
                              vgh(i)=(G(i))

                                  IF(J.eq.1) THEN
                                        Avg_2(i)=vgh(i)
                                  END IF

                                  IF(J.gt.1) THEN
                                        Avg_2(i)=((J-
1)*Avg_1(i))/J+(vgh(i)/J)
END IF
                              Avg_1(i)=Avg_2(i)
                        END DO

                              DO i=0,N_bin
                                    G(i)=0
                              END DO



 Write(8,6)'THETA','PROB'
  6 Format (a5,2x,a5)
DO i=0,N_bin
      WRITE(8,7) (i+0.0)*1,Avg_1(i)*(L/3)
  7 Format(2(f12.6,2x))
END DO
```

```
1 FORMAT(4X,A10,10X,A10)
2 FORMAT(F15.8,5X,F15.8)
3 FORMAT(I3,9X,F9.6,7X,F9.6,7X,F9.6)
4 FORMAT(F15.8,5X,F15.8,5X,F15.8)
5 FORMAT(F8.3,5X,I3,5X)


      END PROGRAM
```

Appendix B: Visual Fortran code used to calculate the one-dimensional density profiles, perpendicular to the nanosheets' surfaces, along Z-axis

```
PROGRAM ONEDENPROFz

IMPLICIT NONE

INTEGER j, p, ik, k, n_atom, m, atom_ID, mole_ID , atom_type,
n_frame, N, N_bin, ig, q,a, ID_mole, l, i, D_ATOM_1, D_ATOM_2
,D_ATOM_3, KK, N_part, T_Skip

REAL Xt, Yt, Zt, R_bin, box, r,  V_l, Avg_d, Nid,  RZ,  RX, RY, AD,
Vx, Vy, Vz, zbot, top, bot, peak

REAL, ALLOCATABLE::                X(:) , Y(:) , Z(:)

REAL, ALLOCATABLE::                G(:) , Avg_1(:) , Avg_2(:)

n_frame =1001
T_Skip = 0
n_atom = 1152
R_bin = 0.1
N_bin = 277
top = 27.72
bot = 0

ALLOCATE( X(1:n_atom) , Y(1:n_atom) , Z(1:n_atom)  )

ALLOCATE( G(0:N_bin), Avg_1(0:N_bin) , Avg_2(0:N_bin)  )

    DO I = 1, n_atom

        X(I)=0; Y(I)=0; Z(I)=0

    END DO


    DO I = 0, N_bin


            G(i)=0

            Avg_1(i)=0

            Avg_2(i)=0

    END DO

OPEN(unit=1, file='XIII-2-1001F.xyz' , status='old')

OPEN(unit=3, file='XIII-2-DEN-Z.data', status='unknown')


    DO I=1, T_Skip
```

```
        DO K=1, n_atom +2
            READ (1,*)
        END DO
        WRITE (*,*) i
    END DO
    DO K=1,n_frame  - T_Skip

      IF ( (K.EQ.1) .OR. (MOD(K,1).EQ.0) ) THEN
                WRITE(*,*) K
            END IF
            DO I=0,N_bin

                    G(i) = 0

            END DO
        DO j=1,2
            READ (1,*)
        END DO
        ik=0

        DO KK=1,n_atom
            READ (1,*) atom_type, Xt, Yt, Zt

                IF ((Xt .GE. 0) .AND. (Xt .LE. 27.72) .AND. (Yt .GE.
0) .AND. (Yt .LE. 27.72) .AND. (Zt .GE. 0) .AND. (Zt .LE. 27.72))
then

                        ik=ik+1

                                X(ik)=Xt*0.90856      ;
      Y(ik)=Yt*0.90856  ;     Z(ik)=Zt*0.90856

                    END IF

          END DO

          N_part=ik

        DO I=0, N_bin
```

```
            DO L = 1, N_part
                IF ( X(L) .LE. ((I+1)*R_bin) .AND. (X(L) .GE.
I*R_bin) ) THEN
                    ig = NINT(Z(L)/R_bin)
                    G(ig) = G(ig) + 1
                END IF
            END DO
        END DO
        DO I=0,N_bin
                    IF (K.EQ.1) THEN
                            Avg_2(i)=G(i)
                      END IF
                      IF (K.GT.1) THEN
                            Avg_2(i)=((k-1)*Avg_1(i))/k  +  ( G(i)/k
)
                      END IF
                        Avg_1(i)=Avg_2(i)
            END DO
    END DO

    WRITE (3,*)  'Z', 'Density'
    DO I=0, N_bin
        RY = (i)*R_bin
                AD = Avg_1(i)/(R_bin)
                Write (3,*)  RY, AD
    END DO
    WRITE (*,*) 'R_bin' , R_bin
      1 Format (21X, I5,  F12.5,  F16.5,  F12.5)
END PROGRAM
```

Appendix C: Visual Fortran code used to calculate the two-dimensional density profiles, parallel to the nanosheets' surfaces

```
PROGRAM TWODDENPROFXY

IMPLICIT NONE

INTEGER j, p, ik, k, n_atom, m, atom_ID, mole_ID , atom_type,
n_frame, N, N_bin, ig, q,a, ID_mole, l, i, D_ATOM_1, D_ATOM_2
,D_ATOM_3, KK, N_part, T_Skip

REAL Xt, Yt, Zt, R_bin, box, r,  V_l, Avg_d, Nid, RZ, RX, RY, AD,
Vx, Vy, Vz, zbot, top, bot, peak, xi, yi, zi, xf, yf,zf

REAL, ALLOCATABLE::                X(:) , Y(:) , Z(:)

REAL, ALLOCATABLE::                G(:, :) , Avg_1( :, :) , Avg_2(
:, :)

n_frame = 1000
T_Skip = 0
n_atom = 144
R_bin = 0.5
N_bin = 51
yf = 27.72
yi = 0
xf = 27.72
xi = 0
zf = 27.72
zi = 13.86

ALLOCATE( X(1:n_atom) , Y(1:n_atom) , Z(1:n_atom)  )

ALLOCATE( G(0:N_bin, 0:N_bin), Avg_1(0:N_bin, 0:N_bin) ,
Avg_2(0:N_bin, 0:N_bin)  )

    DO I = 1, n_atom

        X(I)=0; Y(I)=0; Z(I)=0

    END DO


    DO I = 0, N_bin

        DO J = 0, N_bin

            G(i,j)=0

            Avg_1(i,j)=0

            Avg_2(i,j)=0

        END DO
```

```
    END DO
OPEN(unit=1, file='XII-F-3-1000F.xyz' , status='old')
OPEN(unit=3, file='XII-F-3-DEN-XY-TOP.data', status='unknown')

    DO I=1, T_Skip
        DO K=1, n_atom +2
            READ (1,*)
        END DO
        WRITE (*,*) i
    END DO
    DO K=1,n_frame  - T_Skip

      IF ( (K.EQ.1) .OR. (MOD(K,1).EQ.0) ) THEN
                WRITE(*,*) K
            END IF
            DO I=0,N_bin
                DO J=0, N_bin
                    G(i,j) = 0
                END DO
            END DO
        DO j=1,2
            READ (1,*)
        END DO
        ik=0
        WRITE (2,*) 5148
        WRITE (2,*)
        DO KK=1,n_atom
            READ (1,*) atom_type, xt, yt, zt

                IF (( Xt .GE. xi) .AND. (Xt .LE. xf) .AND.( Yt .GE.
yi) .AND. (Yt .LE. yf) .AND. (Zt .GE. zi) .AND. (Zt .LE. zf)) THEN
```

```
                        ik=ik+1

                                X(ik)=Xt*0.90856      ;
      Y(ik)=Yt*0.90856  ;     Z(ik)=Zt*0.90856


                      END IF

          END DO

          N_part=ik

        DO I=0, N_bin

            DO L = 1, N_part

                IF ( Y(L) .LE. ((I+1)*R_bin) .AND. (Y(L) .GT.
I*R_bin) ) THEN

                    ig = NINT(X(L)/R_bin)

                    G(i,ig) = G(i,ig) + 1

                END IF

            END DO

        END DO


        DO I=0,N_bin

            DO J= 0, N_bin

                    IF (K.EQ.1) THEN

                            Avg_2(i,j)=G(i,j)

                      END IF

                      IF (K.GT.1) THEN

                            Avg_2(i,j)=(k-1)*Avg_1(i,j)/k  +
G(i,j)/k

                      END IF

                        Avg_1(i,j)=Avg_2(i,j)

                  END DO

            END DO

    END DO
```

```
    WRITE (3,*)  'X'         , 'Y'                , 'Atomic number
Density'

    DO I=0, N_bin

        RY = (i)*R_bin

            DO J=0, N_bin

                RX = (j)*R_bin

                AD = Avg_1 (i,j)/(R_bin*R_bin)

                Write (3,*)  RX, RY, AD

            END DO

    END DO

    WRITE (*,*) 'R_bin' , R_bin

      1 Format (21X, I5,  F12.5,  F16.5,  F12.5)

END PROGRAM
```

Appendix D: Visual Fortran code used to count the number of surfactants on the nanosheets' surfaces

```
PROGRAM SURFSORTER

IMPLICIT NONE

INTEGER e,f,d,j, p,ik, k, n_atom, m, ID_atom , n_frame, N, ig, q,a,
ID_mole, L, i, D_ATOM_1, D_ATOM_2 ,D_ATOM_3, skip,ID_typet,
ID_type1,ID_type2, Mole_ID, ix,iy,iz,gap,c

REAL Xt, Yt, Zt, BIN_SIZE, Box, r, Dist, V_1, RHO, Nid, XR,YR,ZR,xu,
yu, zu,vxt,vyt,vzt,Box_Lx,Box_Hx, Box_Ly,Box_Hy,Box_Lz,Box_Hz

REAL, ALLOCATABLE::                X(:,:) , Y(:,:) , Z(:,:)
INTEGER, ALLOCATABLE::      ID_type(:,:)!, ik(:)

n_frame  = 27
n_atom   = 2662
Skip     = 26


ALLOCATE( X(1:(n_frame-Skip),1:n_atom) , Y(1:(n_frame-
Skip),1:n_atom) , Z(1:(n_frame-Skip),1:n_atom), ID_type(1:(n_frame-
Skip),1:n_atom) )

DO d = 1 , n_frame-Skip

   DO c = 1, n_atom

        X(d,c)=0; Y(d,c)=0; Z(d,c)=0 ; ID_type(d,c)=0 ; ik = 0

   END DO

END DO

OPEN(unit=1, file='YIII-F-2-27F.xyz', status='old')

OPEN(unit=2, file='DUPLICATE-YIII-F-2-27F-TOP.data',
status='unknown')

OPEN(unit=3, file='H-COUNT-YIII-F-2-27F-TOP.data', status='unknown')

Do e =1, skip

   DO f =1, n_atom + 2

      READ (1,*)

   END DO

END DO


DO i=1,n_frame - skip
```

```
   IF ( (i.EQ.1) .OR. (MOD(i,1).EQ.0) ) THEN

         WRITE(*,*) 'frame', i

   END IF

                READ (1,*)
                READ (1,*)

         DO k=1,n_atom

            READ(1,*)ID_typet,Xt, Yt, Zt


             IF ((Xt .GE. 0) .AND. (Xt .LE. 27.72) .AND. (Yt .GE. 0)
.AND. (Yt .LE. 27.72) .AND. (Zt .GE. 13.86) .AND. (Zt .LE. 27.72))
then

                   IF (ID_typet .EQ. 2) THEN

                    ik = ik+1

                  END IF

                 WRITE (2,2) ID_typet, Xt, Yt, Zt

               2 FORMAT(I1,5X,F15.8,5X,F15.8,5X,F15.8)

                 END IF


           END DO

         WRITE(3,*) 'H-COUNT =',ik/2,
(ik/((27.72*0.90856)*(27.72*0.90856)*(27.72*0.90856)))/2

END DO


END PROGRAM
```

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Proceedings:

1. Patsinsiri, W.; Suttipong M.; Striolo A.; and Kitiyanan B. (2013, April 23) Mesoscopic Simulation of Sodium Dodecyl Sulfate Aggregates on Graphene Nanosheets. Proceedings of The 4th Research Symposium on Petrochemical and Materials Technology and the 19th PPC Symposium on Petroleum, Petrochemicals, and Polymers, Bangkok, Thailand.

Presentations:

1. Patsinsiri, W.; Suttipong M.; Striolo A.; and Kitiyanan B. (2013, July 7) Mesoscopic Simulation of Sodium Dodecyl Sulfate Aggregates on Graphene Nanosheets. Paper presented at The 33rd International Conference on Solution Chemistry, Kyoto, Japan.