Supporting information for:

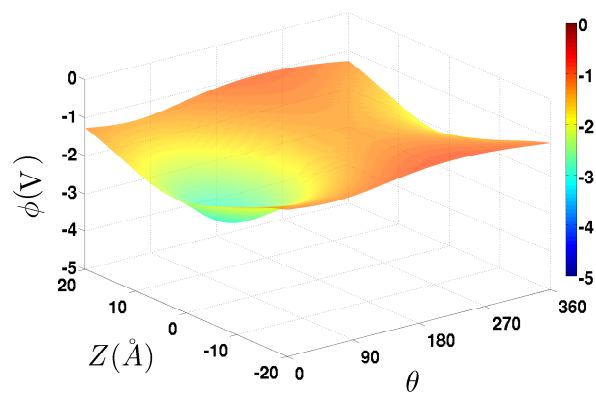# Electrostatics of DNA Nucleotides-Carbon Nanotube Hybrids Evaluated From QM:MM Simulations

Morteza Chehel Amirani and Tian Tang[*]
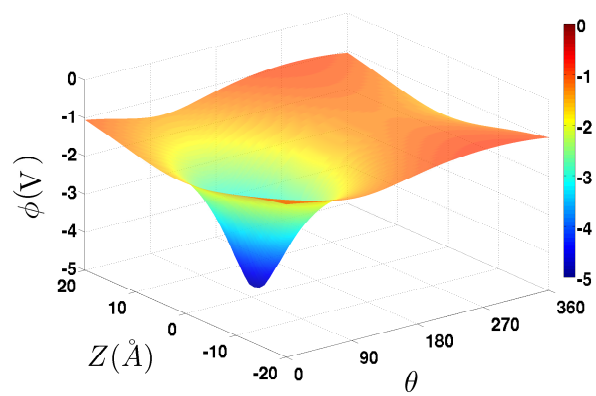
Department of Mechanical Engineering, University of Alberta, Edmonton, AB, Canada
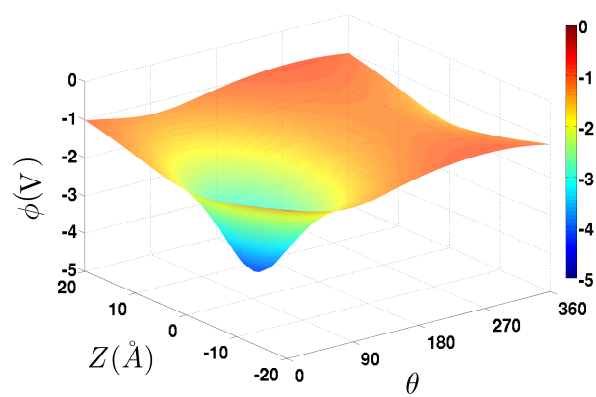
E-mail: tian.tang@ualberta.ca
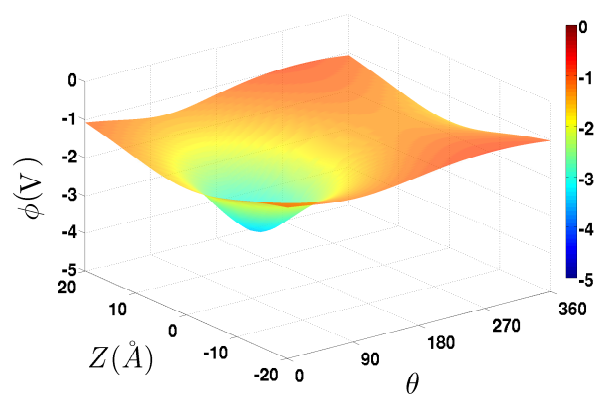

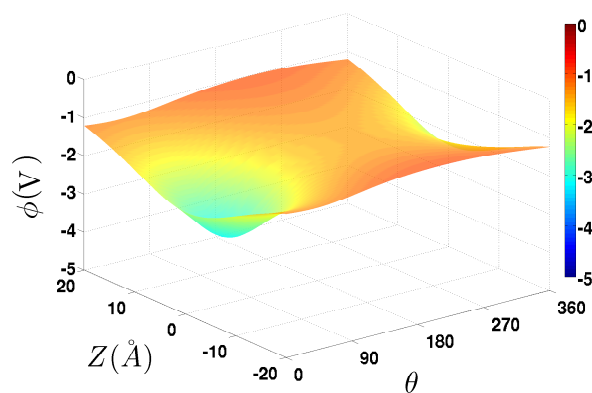[*]To whom correspondence should be addressed
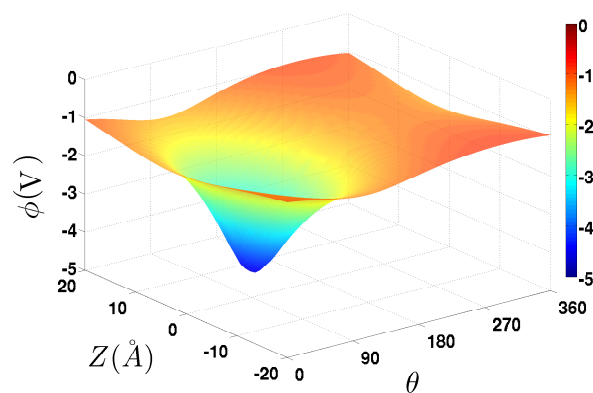
(a) AMP-(7,0) CNT

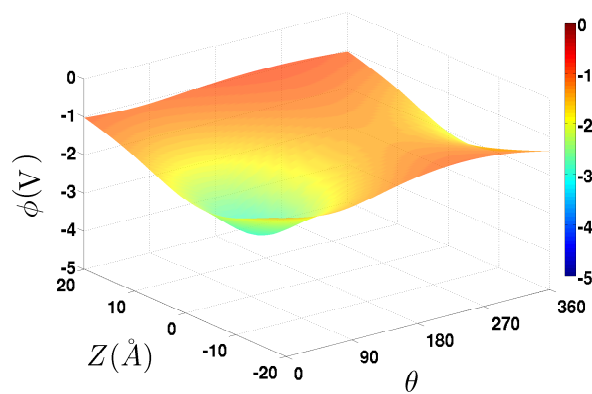(b) AMP-(4,4)CNT

(c) CMP-(7,0) CNT
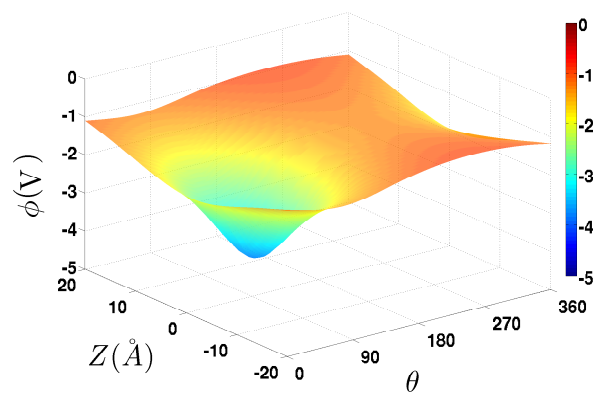
(d) CMP-(4,4)CNT

(e) GMP-(7,0) CNT

(f) GMP-(4,4) CNT
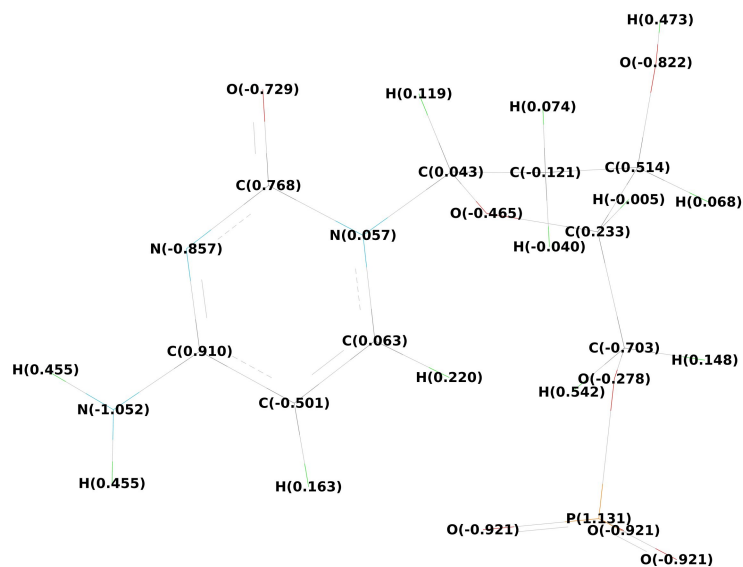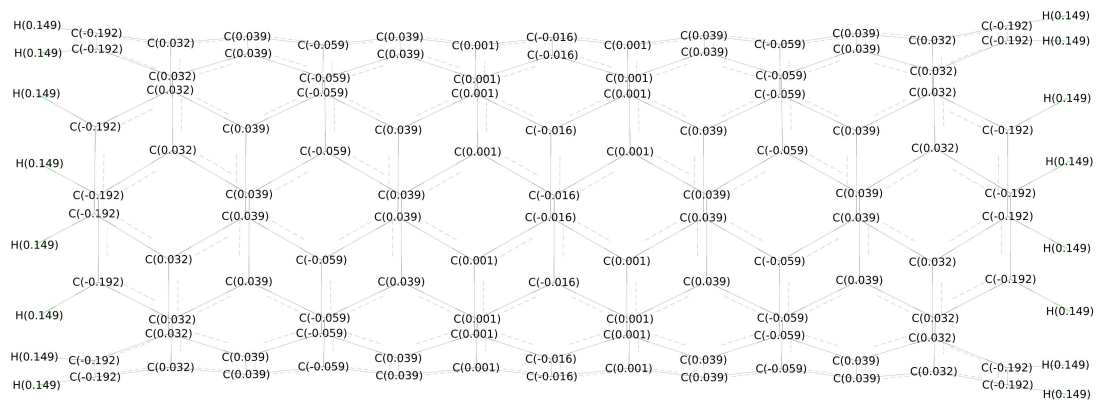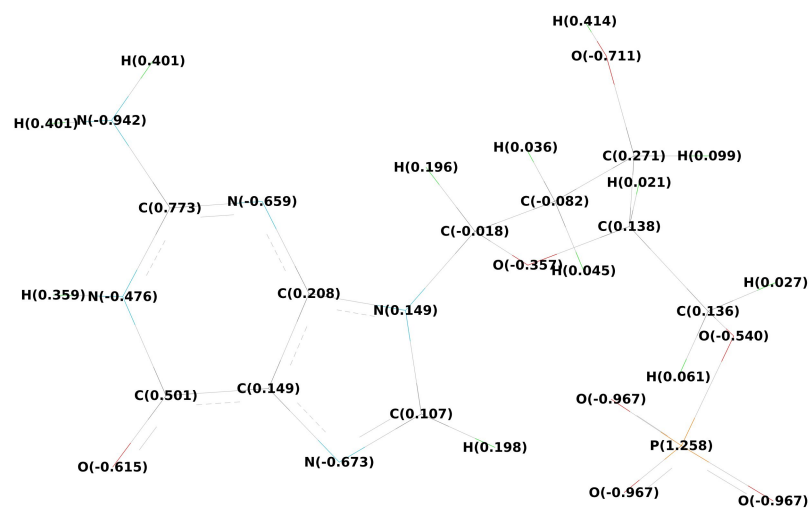

(g) TMP-(7,0) CNT

(h) TMP-(4,4) CNT

Figure S1: Distribution of the electrostatic potential ϕ as a function of Z and θ. The radial distance is fixed at r=15 Å.
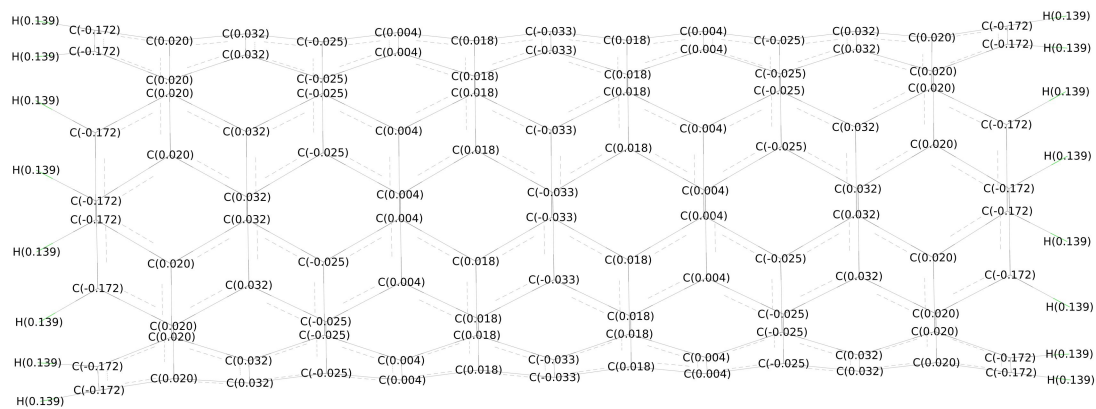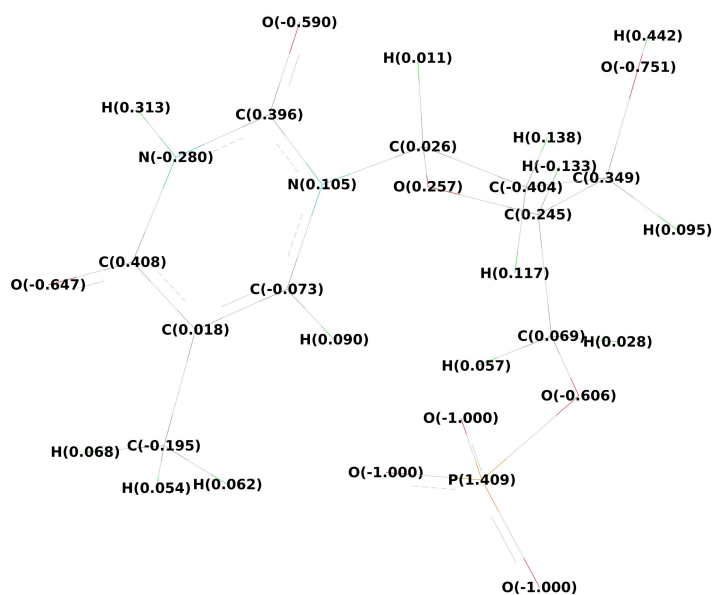
(a)

H(0.384)
O(-0.739)
H(0.043)
H(0.280) H(0.204) C(0.425) H(0.082)
C(0.667) N(-0.849) H(0.065)
C(-0.587)
N(-0.893) C(0.050) C(0.020)
C(0.386) O(-0.358)
N(0.143) H(0.213)
H(0.070)
C(0.050)
C(0.844) C(0.032) O(-0.569)
C(0.337) H(0.101)
H(0.423) N(-0.999) N(-0.751) H(0.125) O(-0.986)
H(0.423) P(1.362)
O(-0.986)
O(-0.986)

(b)

H(0.163) C(-0.180) C(0.024) C(0.021) C(-0.027) C(0.003) C(0.009) C(-0.025) C(0.009) C(0.003) C(-0.027) C(0.021) C(0.024) C(-0.180) H(0.163)
H(0.163) C(0.024) C(0.021) C(-0.027) C(0.003) C(0.009) C(0.009) C(0.003) C(-0.027) C(0.021) C(0.024) H(0.163)
H(0.163) C(-0.180) C(-0.180) C(0.021) C(-0.027) C(0.003) C(-0.025) C(0.009) C(0.003) C(-0.027) C(0.021) C(0.024) C(-0.180) C(-0.180) H(0.163)
C(0.021) C(0.003) C(-0.025)
C(0.024) C(-0.027) C(0.009) C(0.024)

C(-0.180) C(0.021) C(0.003) C(-0.025) C(0.003) C(0.021) C(-0.180)
H(0.163) C(0.024) C(-0.027) C(0.009) C(0.009) C(-0.027) C(0.024) H(0.163)
H(0.163) C(0.024) C(-0.027) C(0.009) C(0.009) C(-0.027) C(0.024) H(0.163)
C(-0.180) C(0.021) C(0.003) C(-0.025) C(0.003) C(0.021) C(-0.180)

C(0.024) C(0.021) C(-0.027) C(0.003) C(0.009) C(-0.025) C(0.009) C(0.003) C(-0.027) C(0.021) C(0.024)
H(0.163) C(-0.180) C(0.021) C(0.003) C(0.021) C(-0.180) H(0.163)
H(0.163) C(0.024) C(-0.027) C(0.009) C(0.009) C(-0.027) C(0.024) H(0.163)
H(0.163) C(-0.180) C(0.024) C(0.021) C(-0.027) C(0.003) C(0.009) C(-0.025) C(0.009) C(0.003) C(-0.027) C(0.021) C(0.024) C(-0.180) H(0.163)
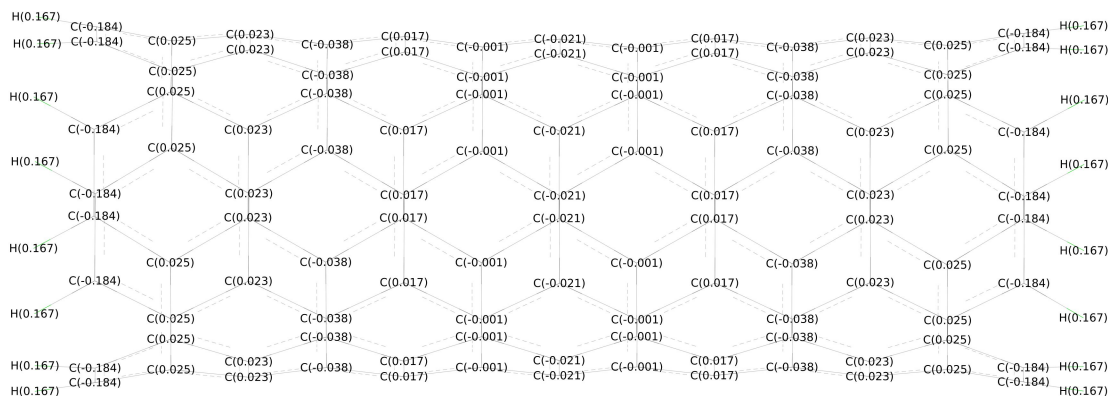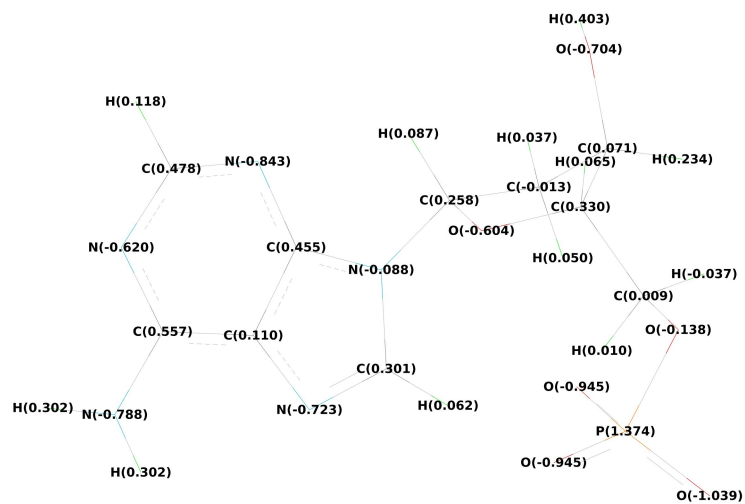
(c)

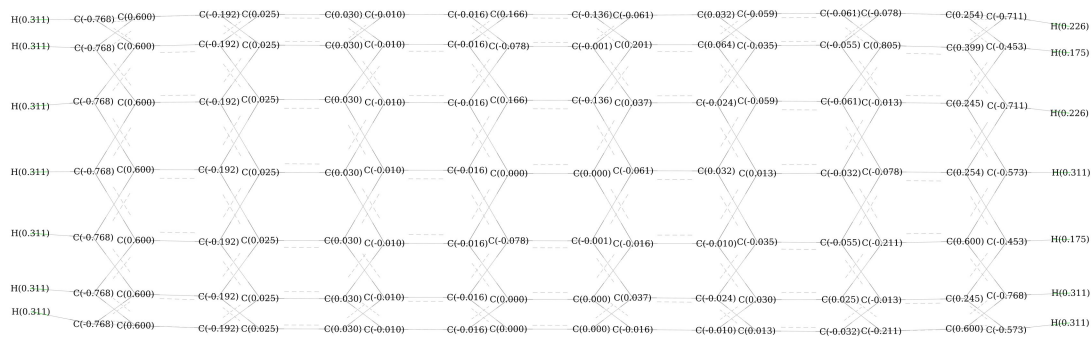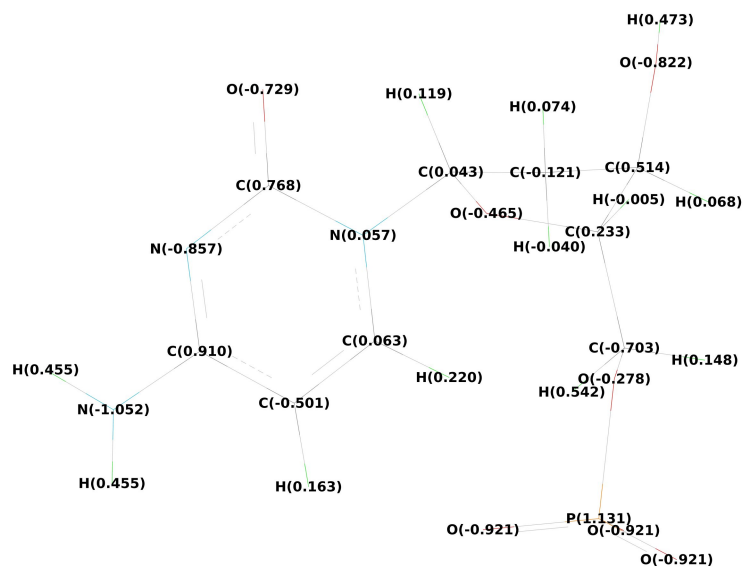
(d)

S5

(e)

(f)

(g)

(h)

Figure S2: Atomic partial charges for: (a) AMP in AMP-(4,4) CNT hybrid, (b) (4,4) CNT in AMP-(4,4) CNT hybrid, (c) CMP in CMP-(4,4) CNT hybrid, (d) (4,4) CNT in CMP-(4,4) CNT hybrid, (e) GMP in GMP-(4,4) CNT hybrid, (f) (4,4) CNT in GMP-(4,4) CNT hybrid, (g) TMP in TMP-(4,4) CNT hybrid, and (h) (4,4) CNT in TMP-(4,4) CNT hybrid. Charges were calculated for the optimized structures using resp approach.
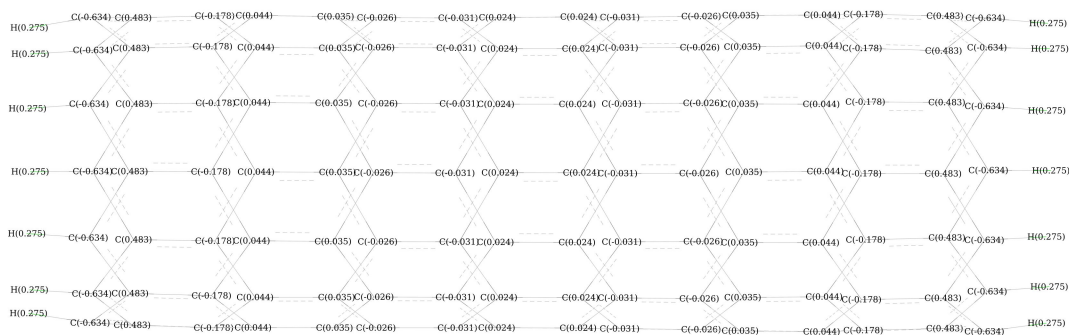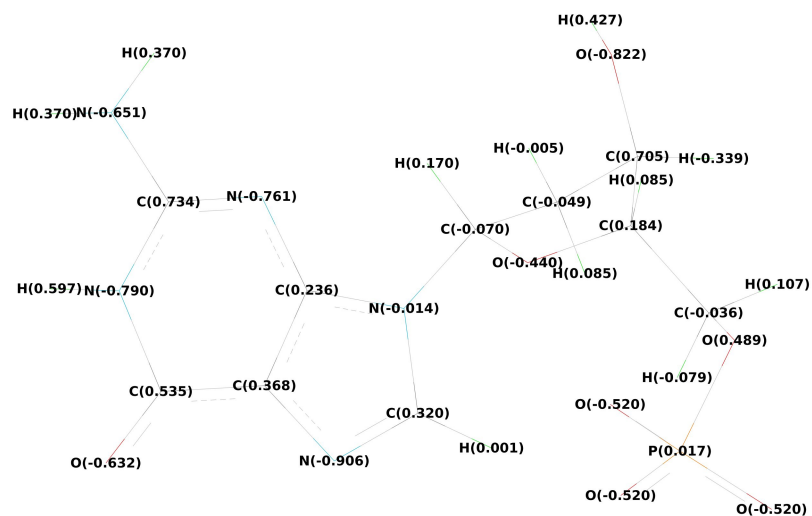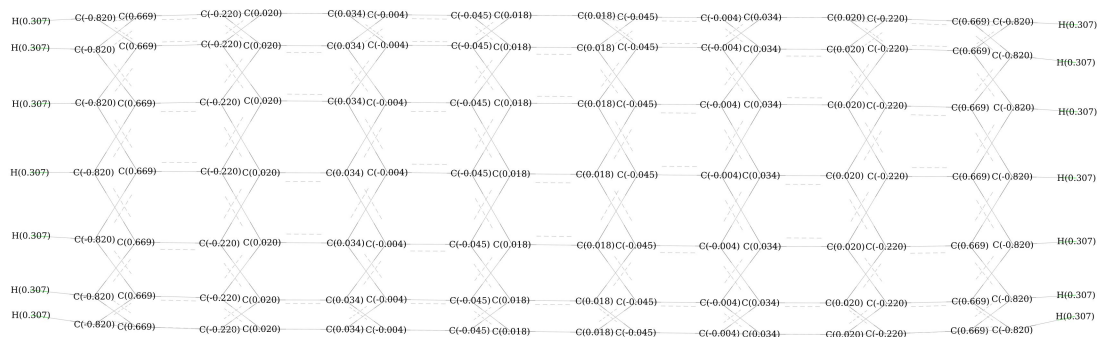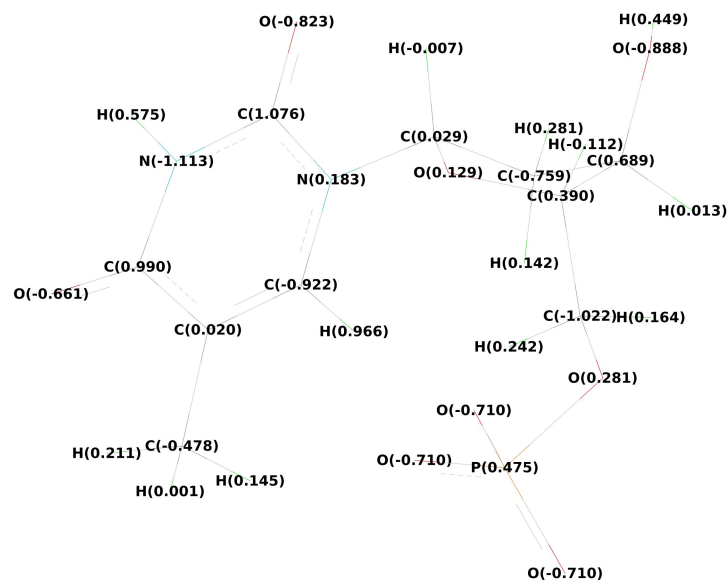
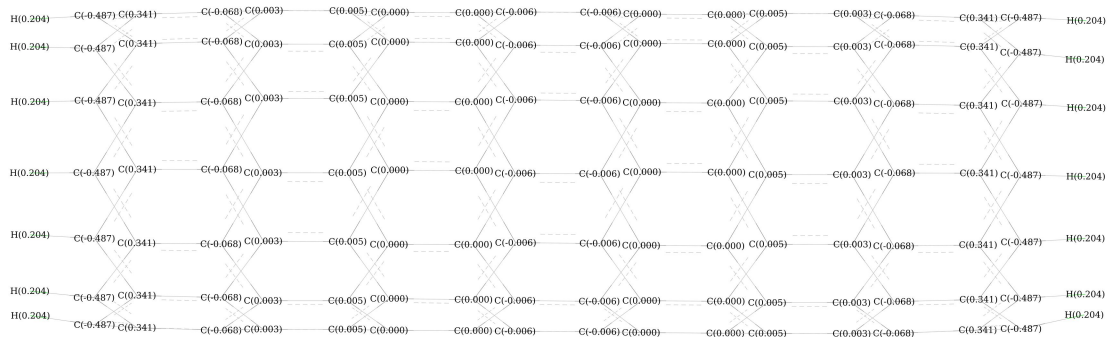(a)

(b)

S8

(c)

(d)

(e)

(f)

(g)

(h)

Figure S3: Atomic partial charges for: (a) AMP in AMP-(7,0) CNT hybrid, (b) (7,0) CNT in AMP-(7,0) CNT hybrid, (c) CMP in CMP-(7,0) CNT hybrid, (d) (7,0) CNT in CMP-(7,0) CNT hybrid, (e) GMP in GMP-(7,0) CNT hybrid, (f) (7,0) CNT in GMP-(7,0) CNT hybrid, (g) TMP in TMP-(7,0) CNT hybrid, and (h) (7,0) CNT in TMP-(7,0) CNT hybrid. Charges were calculated for the optimized structures using resp approach.