Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Title:Interactions, Electronic and Optical properties of Nanographene- Peptide Complexes: A Theoretical Study

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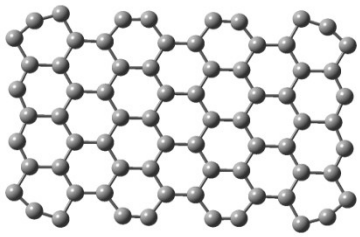
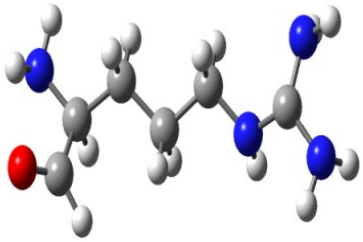
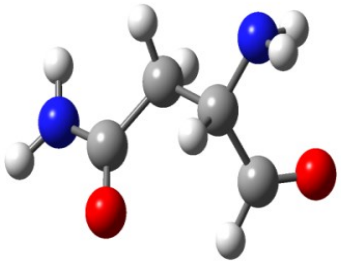
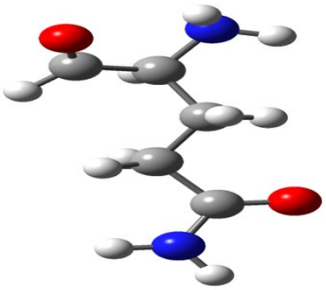
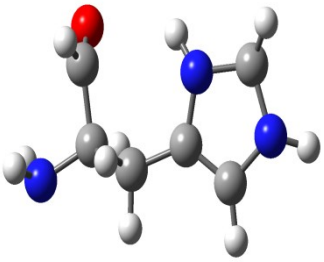
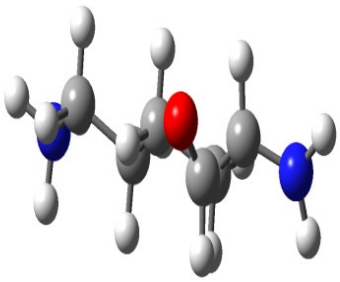
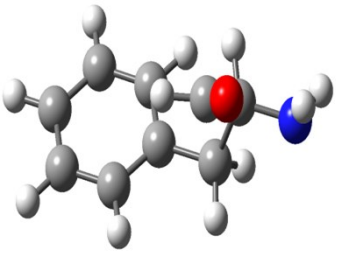
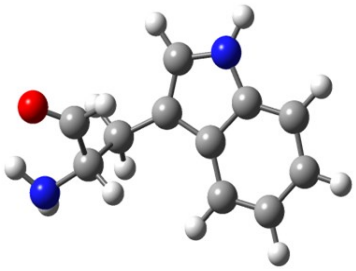
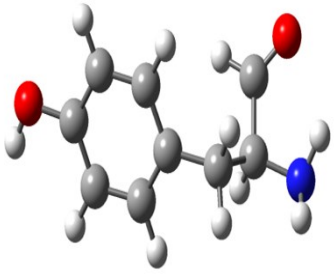
Complexes	B3LYP/6-31G*	M06/6-31G*	B3LYP-D2/6-31G*
nanographene	-2740.32	-2740.36	-2741.24
arg	-531.788	-530.877	-531.988
asn	-416.129	-416.959	-417.329
gln	-455.652	-456.239	-456.488
his-c	-473.131	-473.744	-474.016
lys-c	-421.363	-422.100	-422.242
phe	-479.266	-479.428	-479.504
try	-610.281	-610.700	-611.063
tyr	-553.787	-554.409	-554.724

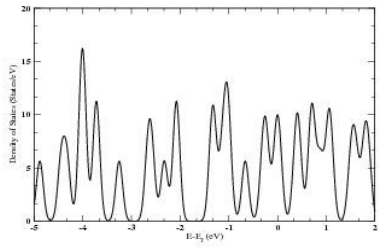
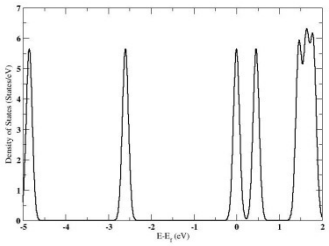
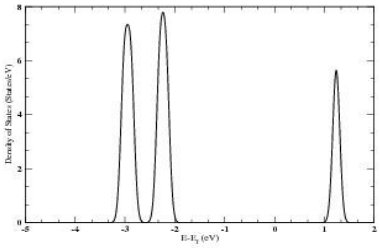
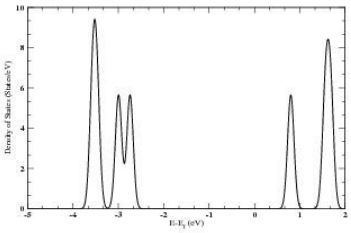
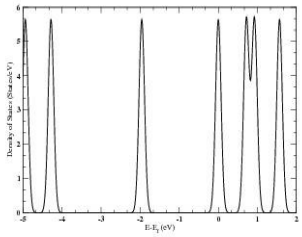
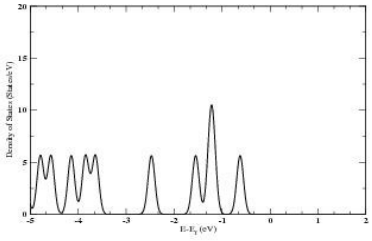
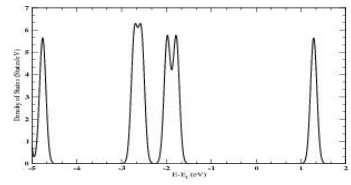
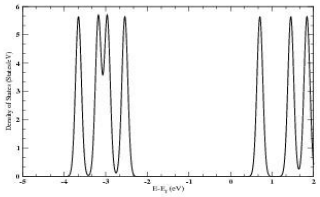
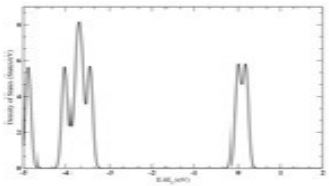
Supplementary Table 1: Optimized energy values for nanographene and all the peptides with three different DFT (a)B3LYP/6-31G*, (b) M06/6-31G* and (c) B3LYP-D2/6-31G* methods.

Complexes	HL Gap (eV)	Dipole moment (Debye)	Polarizability
nanographene	3.86	0.001	474.22
arg	4.23	5.721	66.23
asn	7.11	4.522	32.22
gln	7.31	5.421	49.86
his-c	6.33	3.572	45.37
lys-c	6.70	4.035	54.18
phe	7.21	3.277	52.56
try	6.14	4.843	72.45
tyr	6.72	4.366	66.78

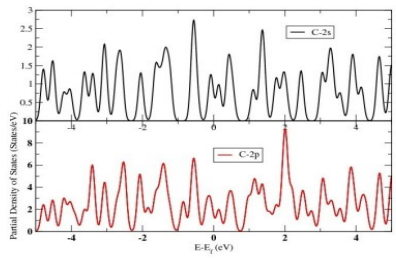
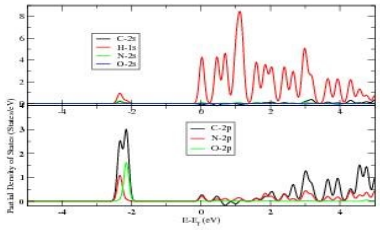
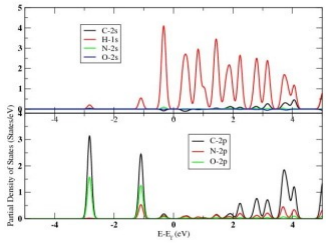
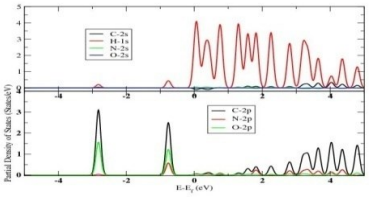
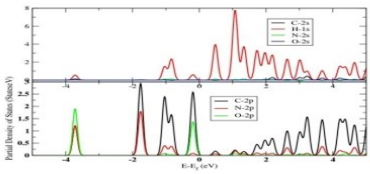
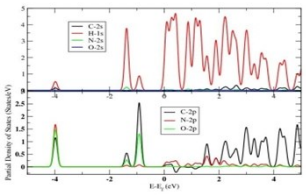
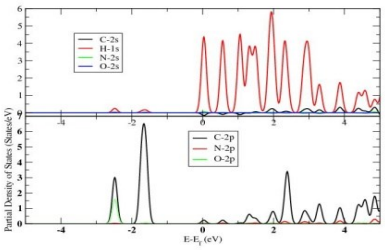
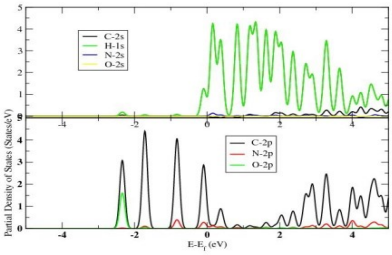
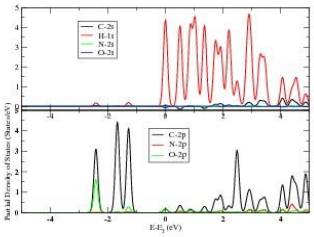
Supplementary Table 2: HL Gap (eV), Dipole moment (Debye) and Polarizability of nanographene(g) and arg, asn, gln, his-c, lys-c, phe, try and tyr peptides in aqueous medium by B3LYP-D2/6-31G*DFT method.

		
nanographene	arginine (arg)	asparagine (asn)
		
glutamine (gln)	histidine (his) -c	lysine (lys)-c
		
phenylalanine (phe)	tryptophan (try)	tyrosine (tyr)

Supplementary Figure 1: Optimized structures of nanographene and peptide complexes in aqueous medium by B3LYP-D2/6-31G* DFT method.

		
nanographene	arginine (arg)	asparagine (asn)
		
glutamine (gln)	histidine (his) -c	lysine (lys)-c
		
phenylalanine (phe)	tryptophan (try)	tyrosine (tyr)

Supplementary Figure 2: Density of States (DOS) graph for nanographene (g) andarg, asn, gln, his-c, lys-c, phe, try and tyr peptides.

		
nanographene	arginine (arg)	asparagine (asn)
		
glutamine (gln)	histidine (his) -c	lysine (lys)-c
		
phenylalanine (phe)	tryptophan (try)	tyrosine (tyr)

Supplementary Figure 3: Partial density of States (PDOS) graph for nanographene (g) and arg, asn, gln, his-c, lys-c, phe, try and tyr peptides.