Electronic Supplementary Information (ESI)

Structural and electronic properties of covalently functionalized 2-aminoethoxy-metallophthalocyanine-graphene hybrid materials: a computational study†

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Table S1 Comparison of the computed isotropic polarizabilities, α (in a.u.) and average hyperpolarizabilities, β (in a.u.) of graphene, AEZnPc, and AEZnPc-graphene using three different meta-hybrid functionals.

System	α			β		
	M06-2X	CAM-B3LYP	wB97XD	M06-2X	CAM-B3LYP	wB97XD
graphene	1165.5	1203.4	1283.9	2.6	2.9	3.9
AEZnPc	649.5	659.0	666.3	1378.8	1388.9	1363.6
AEZnPc-graphene	1801.6	1850.9	1953.6	1926.0	1992.7	1920.8

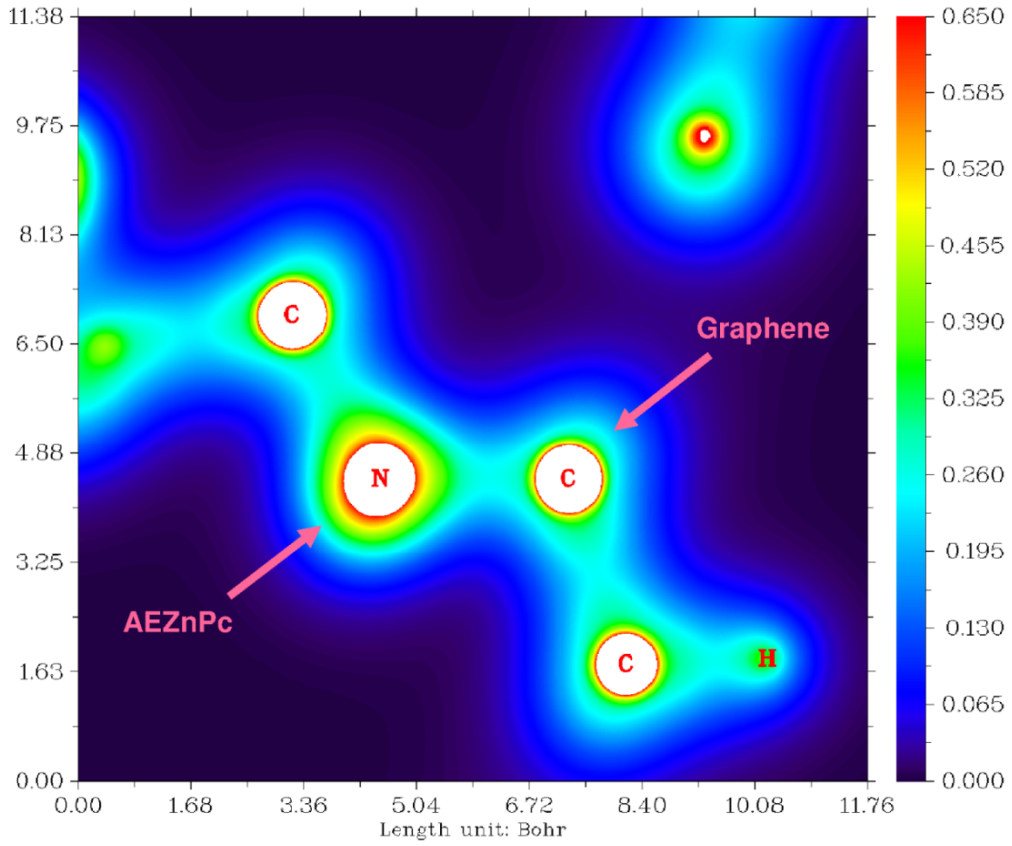

Fig. S1 Color-filled electron density map of AEZnPc-graphene complex.

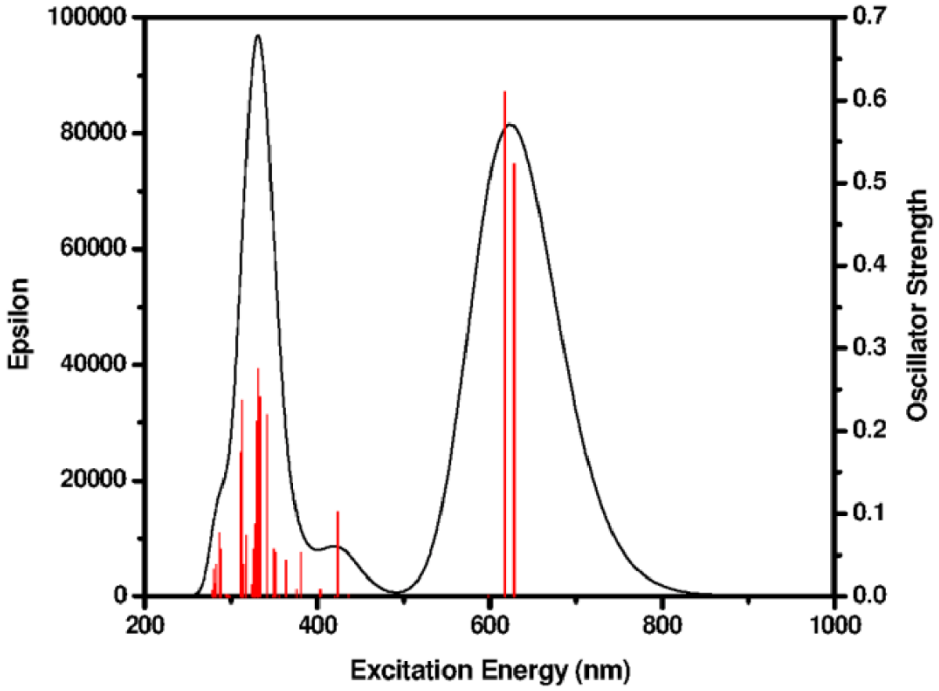

Fig. S2 Computed UV spectra of AENiPc in DMF solvent

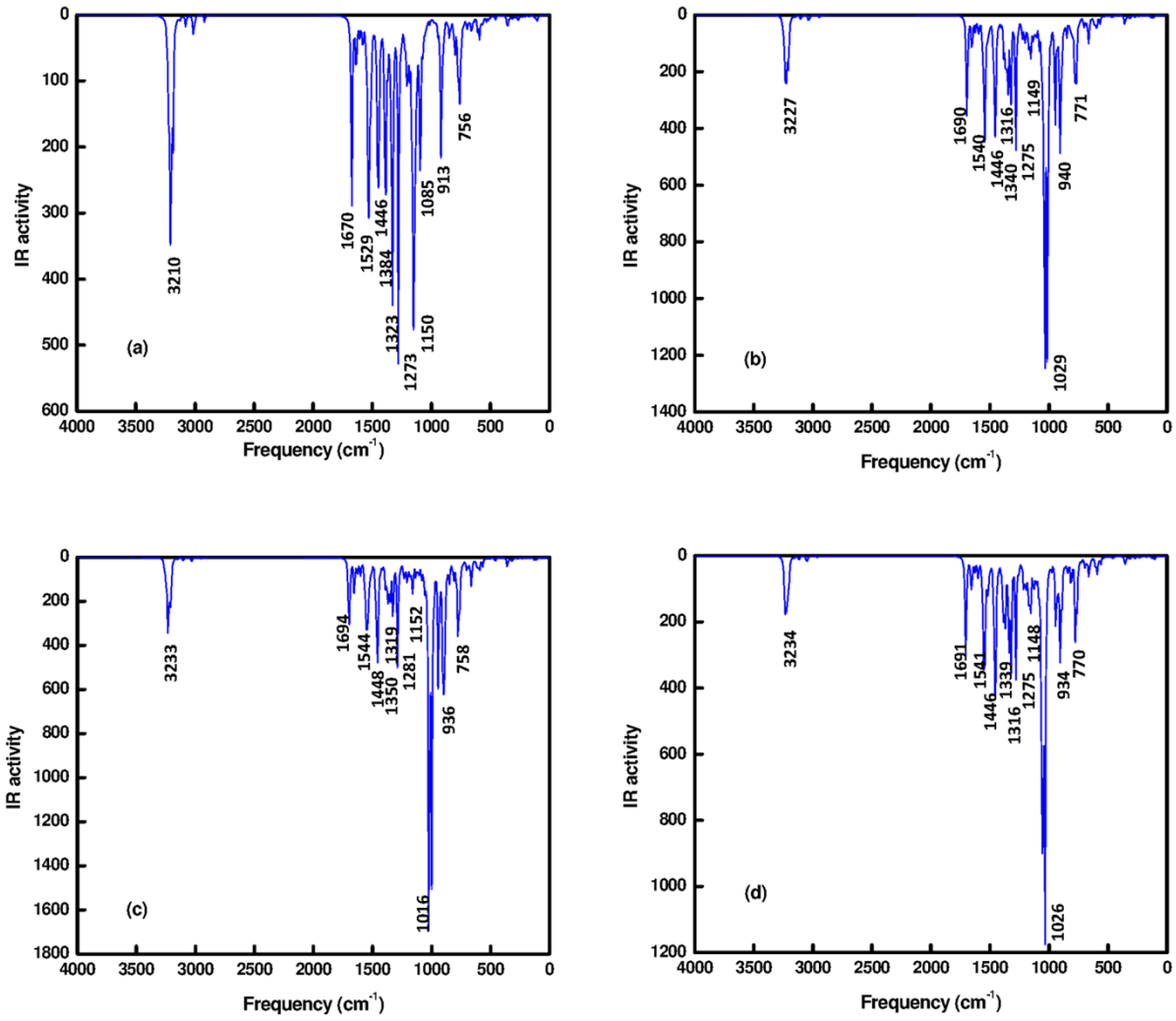

Fig. S3 Computed IR spectra of AEZnPc-graphene using different functionals: (a) B3LYP, (b) CAM-B3LYP, (c) wB97XD, (d) M06-2X

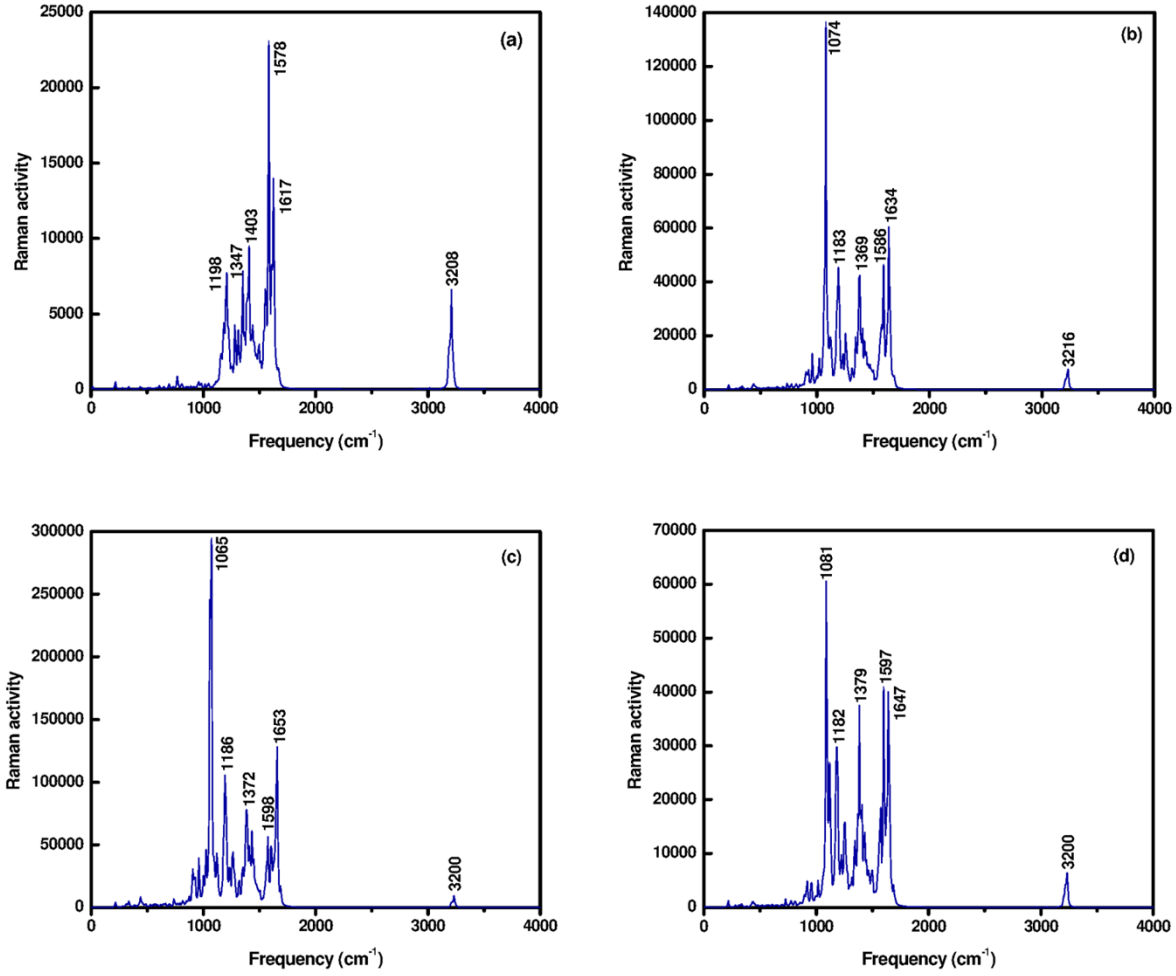

Fig. S4 Computed Raman activity of AEZnPc-graphene using different functionals: (a) B3LYP, (b) CAM-B3LYP, (c) wB97XD, (d) M06-2X