Table S2. Alpha occupied and virtual eigenvalues molecular orbitals coefficients of Co_3O_4@PANI NCs, standard basis set B3LYP function 6-31G(d) (6D, 7F).

Molecular Orbitals Coefficients	**1**	**2**	**3**	**4**	**5**
α-Occupied eigenvalues	-14.32812	-14.32812	-10.20941	-10.20940	-10.17466
	-10.17465	-10.17410	-10.17410	-0.90668	-0.89774
	-0.80948	-0.73249	-0.69872	-0.60804	-0.58221
	-0.51189	-0.51161	-0.48197	-0.47121	-0.42563
	-0.40929	-0.40013	-0.37587	-0.37354	-0.33048
	-0.32513	-0.25726	-0.23748	-0.17066	
α-Virtual eigenvalues	**6**	**7**	**8**	**9**	**10**
	0.01074	0.03880	0.08780	0.08908	0.11430
	0.12220	0.14704	0.18083	0.18171	0.18681
	0.20379	0.25445	0.30014	0.34563	0.34747
	0.35061	0.37271	0.50021	0.53499	0.55337
	0.55775	0.56127	0.59430	0.60627	0.61143
	0.61309	0.62479	0.63963	0.65042	0.67126
	0.69364	0.71857	0.72240	0.78485	0.79040
	0.84096	0.84354	0.85389	0.87076	0.89535
	0.89745	0.90901	0.91581	0.92815	0.93289
	0.99572	1.00209	1.03030	1.03056	1.04276
	1.06882	1.18096	1.20498	1.20528	1.26099
	1.27787	1.36243	1.42075	1.46176	1.46577
	1.49249	1.53027	1.54856	1.55577	1.76815
	1.78424	1.84053	1.84513	1.90312	1.90560
	1.92209	1.97620	1.99227	1.99810	2.06165
	2.07076	2.14177	2.14380	2.15253	2.19695
	2.23276	2.26583	2.32725	2.40982	2.43235
	2.44261	2.50097	2.50862	2.53357	2.60758
	2.62652	2.69164	2.74836	2.83130	2.85219
	2.89215	2.92463	3.12564	3.42906	3.82926
	3.86556	4.09997	4.12816	4.15974	4.34264
	4.40302	4.72957			