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Supporting Information

A new turn in Codon-Anticodon selection through halogen bonds

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Table SIT1 The computed bond parameters along with deformation energy

Base Pairs	Bond	Bond Length (Å)		Deformation in bond lengths (Å)	Deformation energy (kcal/mol)
		Base pair	Monomer		
Ura:Ade	Uracil-N-H	1.039	1.011	0.028	1.06
	Adenine-N-H	1.017	1.005	0.015	
Ura:Ade (Cl)	Uracil-N-Cl	1.704	1.695	0.009	0.17
	Adenine-N-Cl	1.700	1.704	0.004	
Ura:Ade (Br)	Uracil-N-Br	1.871	1.838	0.033	0.77
	Adenine-N-Br	1.833	1.824	0.009	
Ura:Ade (I)	Uracil-N-I	2.096	2.072	0.023	0.90
	Adenine-N-I	2.045	2.045	0.0004	
Ura:Cyt	Uracil-N-H	1.032	1.011	0.021	1.44
	Cytosine-N-H	1.020	1.006	0.014	
Ura:Cyt (Cl)	Uracil-N-Cl	1.702	1.695	0.007	0.27
	Cytosine-N-Cl	1.698	1.701	0.0035	
Ura:Cyt (Br)	Uracil-N-Br	1.860	1.838	0.022	1.02
	Cytosine-N-Br	1.841	1.828	0.013	
Ura:Cyt (I)	Uracil-N-I	2.117	2.072	0.045	2.60
	Cytosine-N-I	2.065	2.048	0.017	
Ura:Gua	Uracil-N-H	1.032	1.011	0.021	1.76
	Guanine-N-H	1.023	1.008	0.015	
Ura:Gua (Cl)	Uracil-N-Cl	1.699	1.695	0.004	0.14
	Guanine-N-Cl	1.705	1.704	0.002	
Ura:Gua (Br)	Uracil-N-Br	1.851	1.838	0.013	0.41
	Guanine-N-Br	1.858	1.846	0.012	
Ura:Gua (I)	Uracil-N-I	2.083	2.072	0.017	0.39
	Guanine-N-I	2.089	2.084	0.005	
Ura:Ura	Uracil-N-H	1.025	1.011	0.014	0.83
	Uracil-N-H	1.025	1.011	0.013	
Ura:Ura (Cl)	Uracil-N-Cl	1.698	1.695	0.003	0.10
	Uracil-N-Cl	1.698	1.695	0.003	
Ura:Ura (Br)	Uracil-N-Br	1.846	1.838	0.008	0.27
	Uracil-N-Br	1.847	1.838	0.008	
Ura:Ura (I)	Uracil-N-I	2.080	2.072	0.008	0.27
	Uracil-N-I	2.078	2.072	0.006	

Table SIT2: The computed interaction energies with and without counter poise correction.

System	Binding Energy in kcal/mol	
	Uncorrected	**BSSE corrected**
Ura:Ade	-14.72	-13.87
Ura:Ade(Cl)	-5.70	-4.82
Ura:Ade(Br)	-5.97	-5.39
Ura:Ade(I)	-9.64	-8.95
Ura:Cyt	-13.47	-12.41
Ura:Cyt(Cl)	-5.63	-4.70
Ura:Cyt(Br)	-7.64	-7.01
Ura:Cyt(I)	-15.14	-14.24
Ura:Gua	-16.51	-15.65
Ura:Gua(Cl)	-5.60	-4.77
Ura:Gua(Br)	-6.25	-5.79
Ura:Gua(I)	-9.18	-8.55
Ura:Ura	-12.34	-11.51
Ura:Ura(Cl)	-4.62	-3.82
Ura:Ura(Br)	-5.07	-4.57
Ura:Ura(I)	-7.65	-7.03

Table SIT3 The topological properties of X---X interactions from AIM analysis

System	Bonds	rho	L(r)	Ellipticity	H(r)	V(r)/G(r)
Ura:Ade (Cl)	Cl---Cl	0.00806	-0.00806	0.08818	0.01055	0.70
Ura:Cyt (Cl)	Cl---Cl	0.00763	-0.00759	0.05652	0.00986	0.69
Ura:Gua (Cl)	Cl---Cl	0.00863	-0.00874	0.11798	0.01153	0.70
Ura:Ura (Cl)	Cl---Cl	0.00814	-0.00815	0.12459	0.01061	0.69
Ura:Ade (Br)	Br---Br	0.01357	-0.01148	0.19299	0.01654	0.77
Ura:Cyt (Br)	Br---Br	0.00760	-0.00582	0.08069	0.00828	0.76
Ura:Gua (Br)	Br---Br	0.01278	-0.01088	0.18019	0.01549	0.76
Ura:Ura (Br)	Br---Br	0.01211	-0.01008	0.18543	0.01435	0.76
Ura:Ade (I)	I---I	0.00980	-0.00657	0.20061	0.01036	0.83
Ura:Cyt (I)	I---I	0.00588	-0.00438	0.18756	0.00620	0.75
Ura:Gua (I)	I---I	0.01117	-0.00765	0.23442	0.01245	0.85
Ura:Ura (I)	I---I	0.01034	-0.00711	0.22521	0.01134	0.84

Table SIT4 The θ_1 and θ_2 angles of X---X interactions

Base Pair	θ_1	θ_2
Ura:Ade (Cl)	123.7	103.3
Ura:Ade (Br)	111.1	96.1
Ura:Ade (I)	127.4	90.3
Ura:Cyt (Cl)	107.3	110.4
Ura:Cyt (Br)	99.82	104.4
Ura:Cyt (I)	92.6	100.3
Ura:Gua (Cl)	107.5	112.2
Ura:Gua (Br)	103.8	106.5
Ura:Gua (I)	96.7	105.9
Ura:Ura (Cl)	109.3	109.1
Ura:Ura (Br)	104.7	104.0
Ura:Ura (I)	102.0	98.1

Figure SIF1 The optimized structures of Uracil : Adenine base pairs

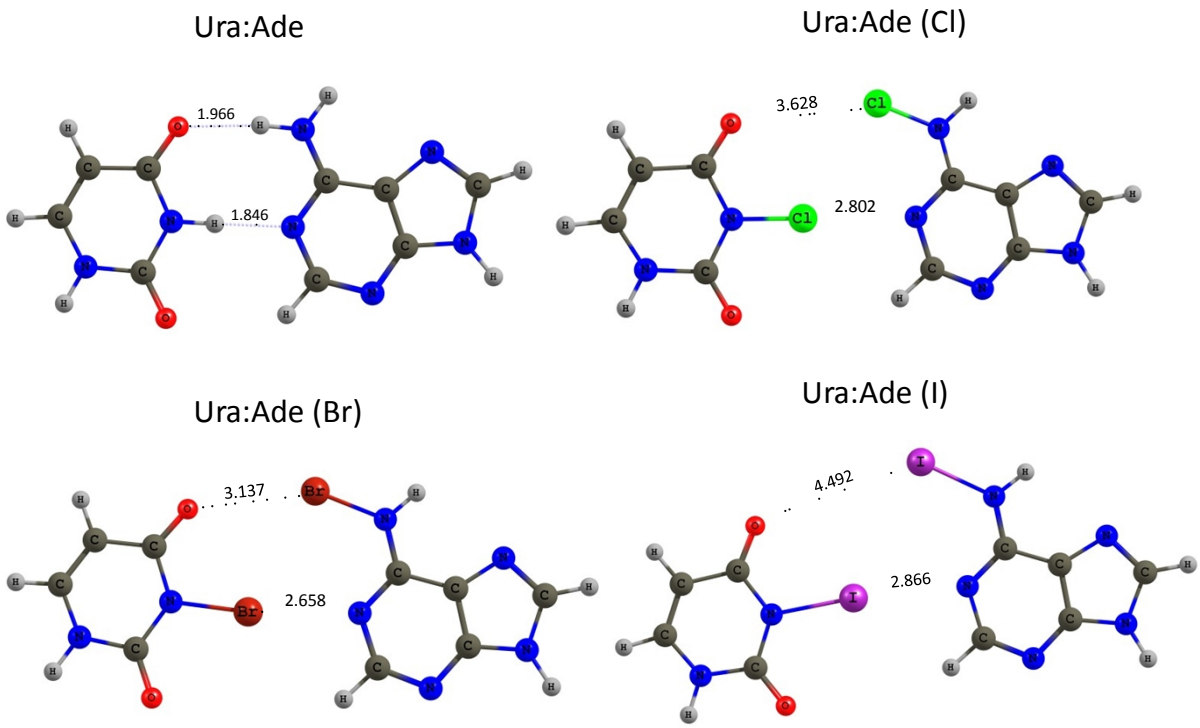

Figure SIF2 The optimized structures of Uracil : Cytosine base pairs

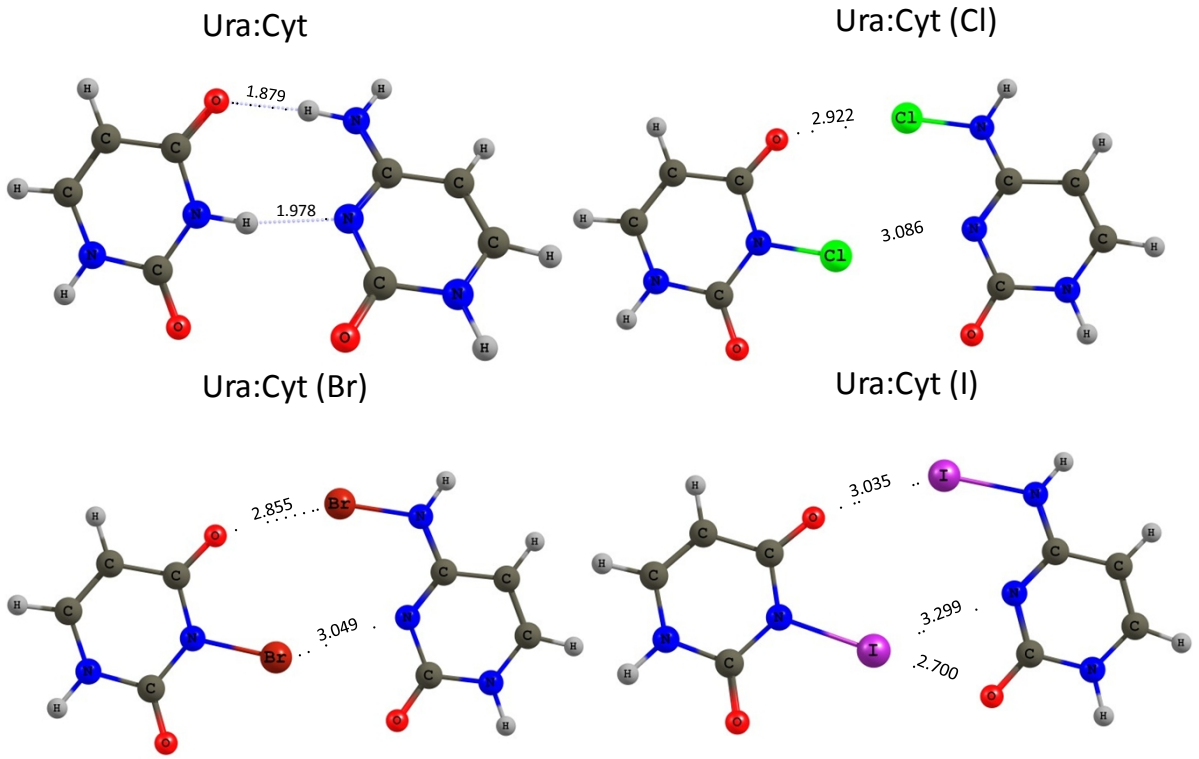

Figure SIF3 The optimized structures of Uracil : Guanine base pairs

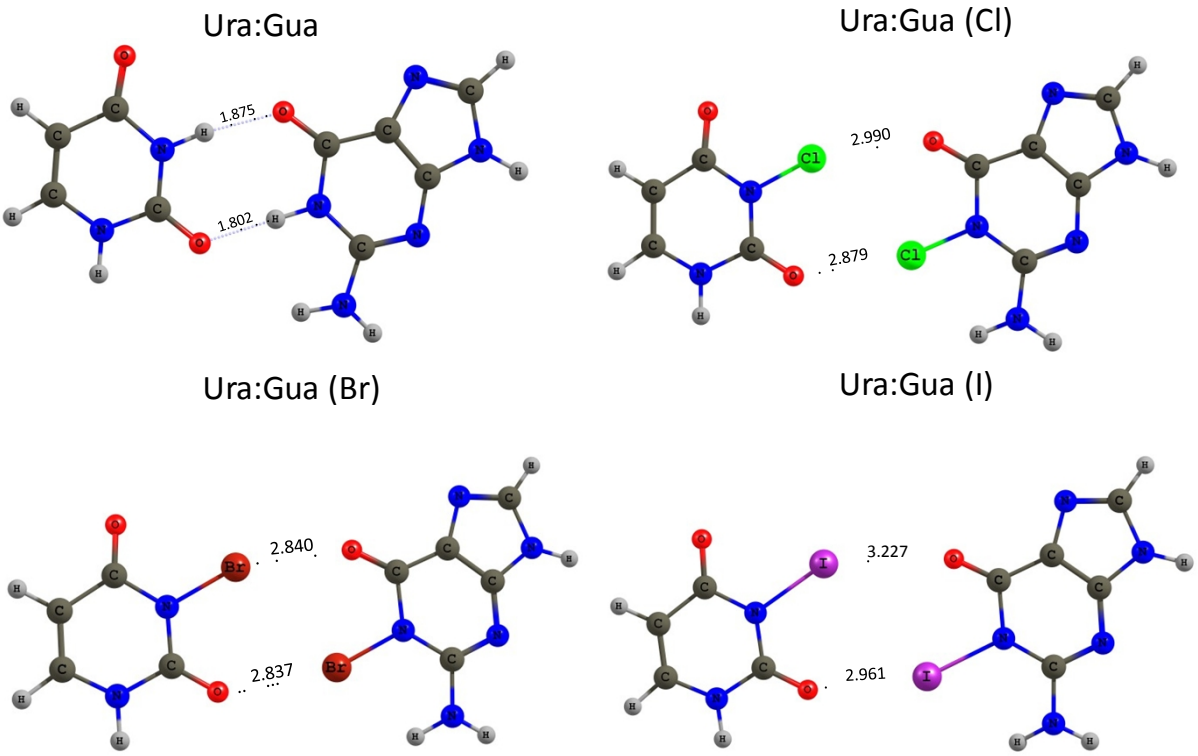

Figure SIF4 The optimized structures of Uracil : Uracil base pairs

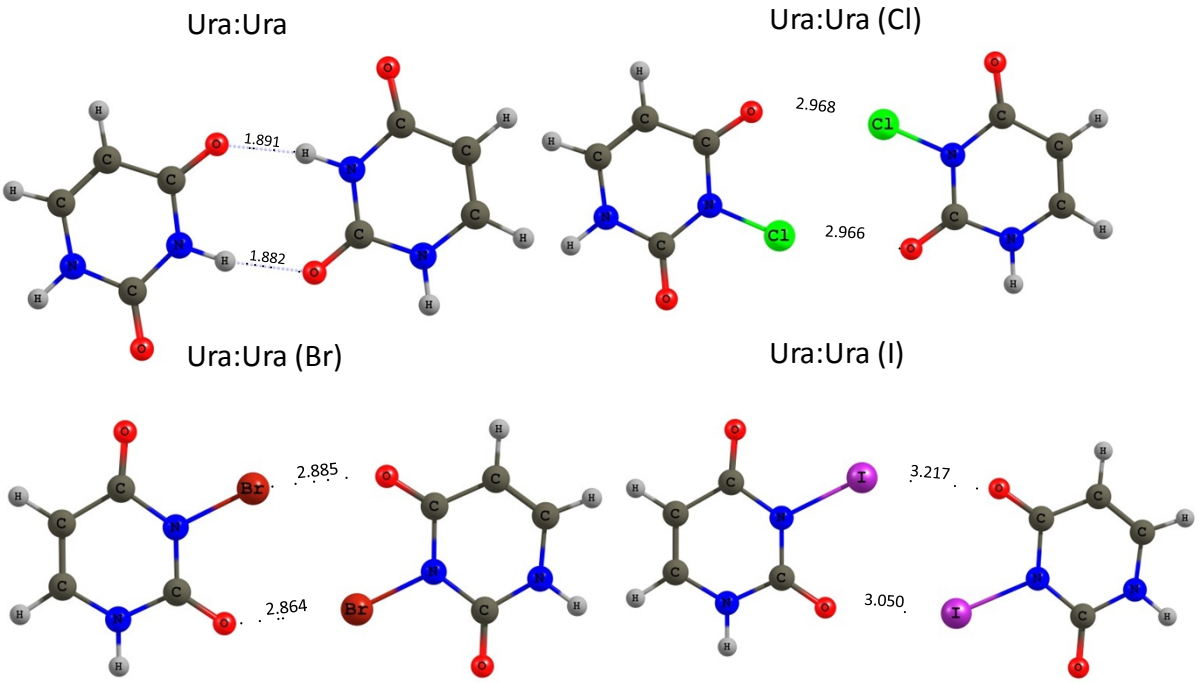

Figure SIF5 The computed electrostatic potential charges at M05-2X level

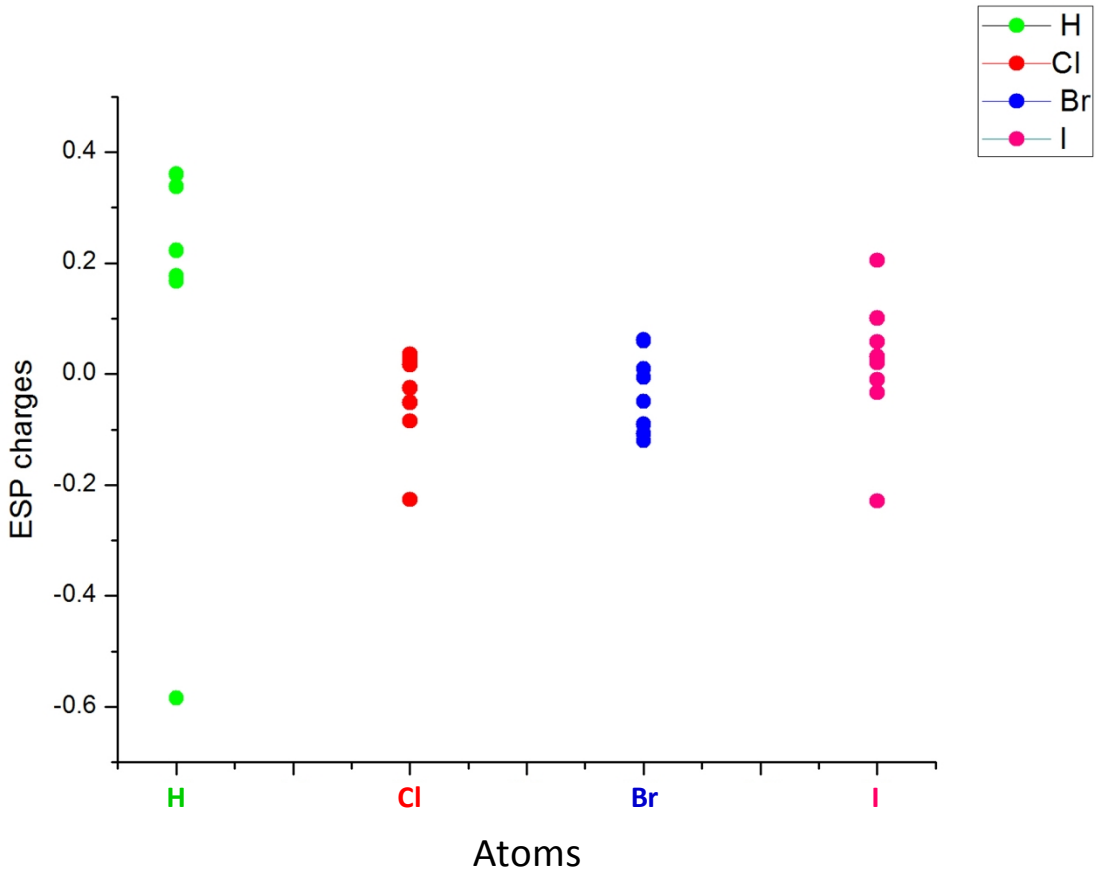

Figure SIF6 The graph of the reduced electron density gradient vs sign of λ_2 in Ura:Ade(X) where X= H, Cl, Br & I

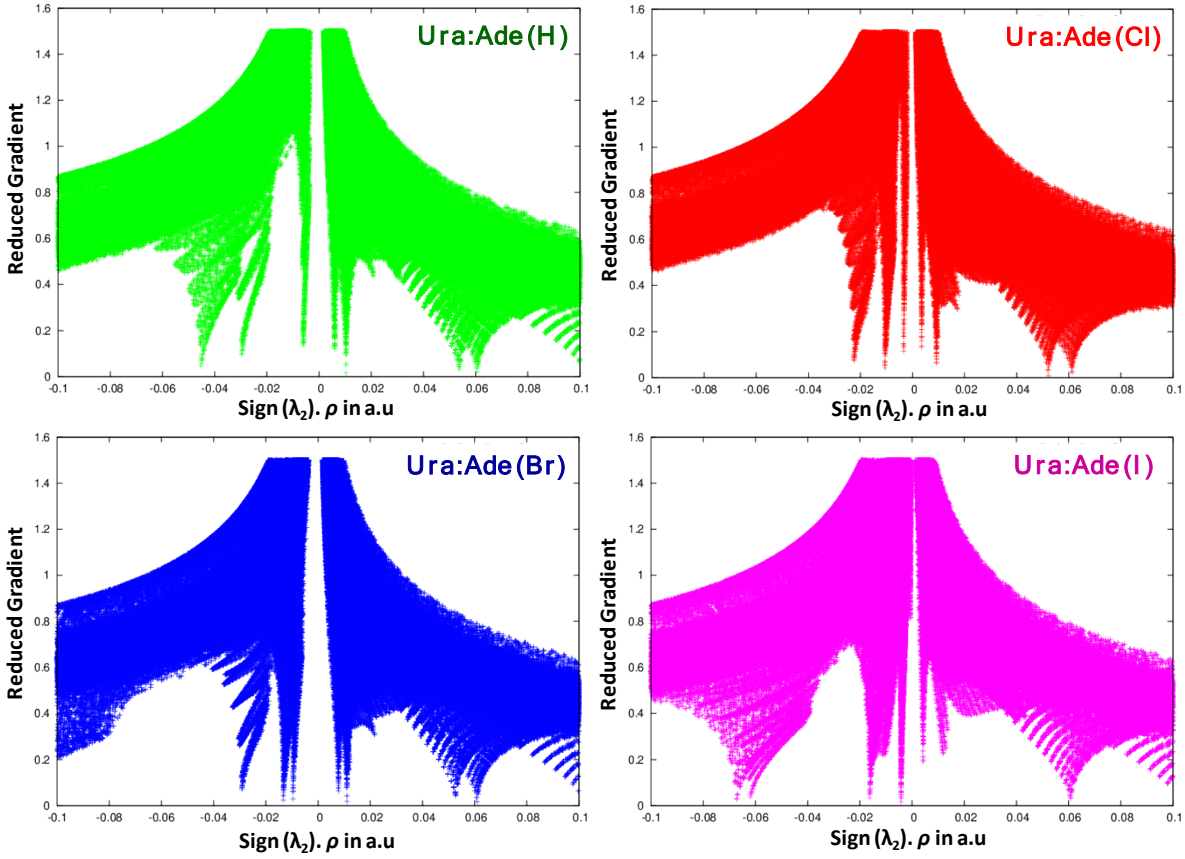

Figure SIF7 The graph of the reduced electron density gradient vs sign of λ_2 in Ura:Cyt(X) where X= H, Cl, Br & I

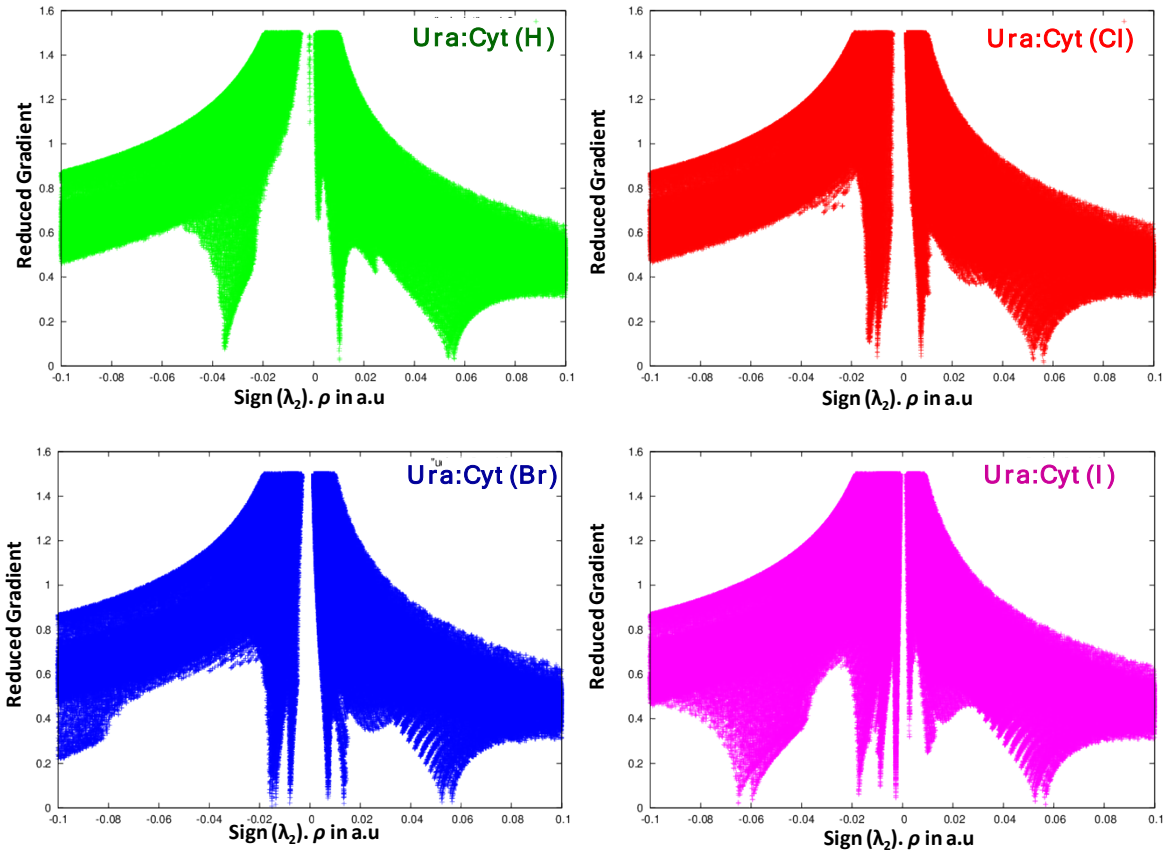

Figure SIF8 The graph of the reduced electron density gradient vs sign of λ_2 in Ura:Gua(X) where X= H, Cl, Br & I

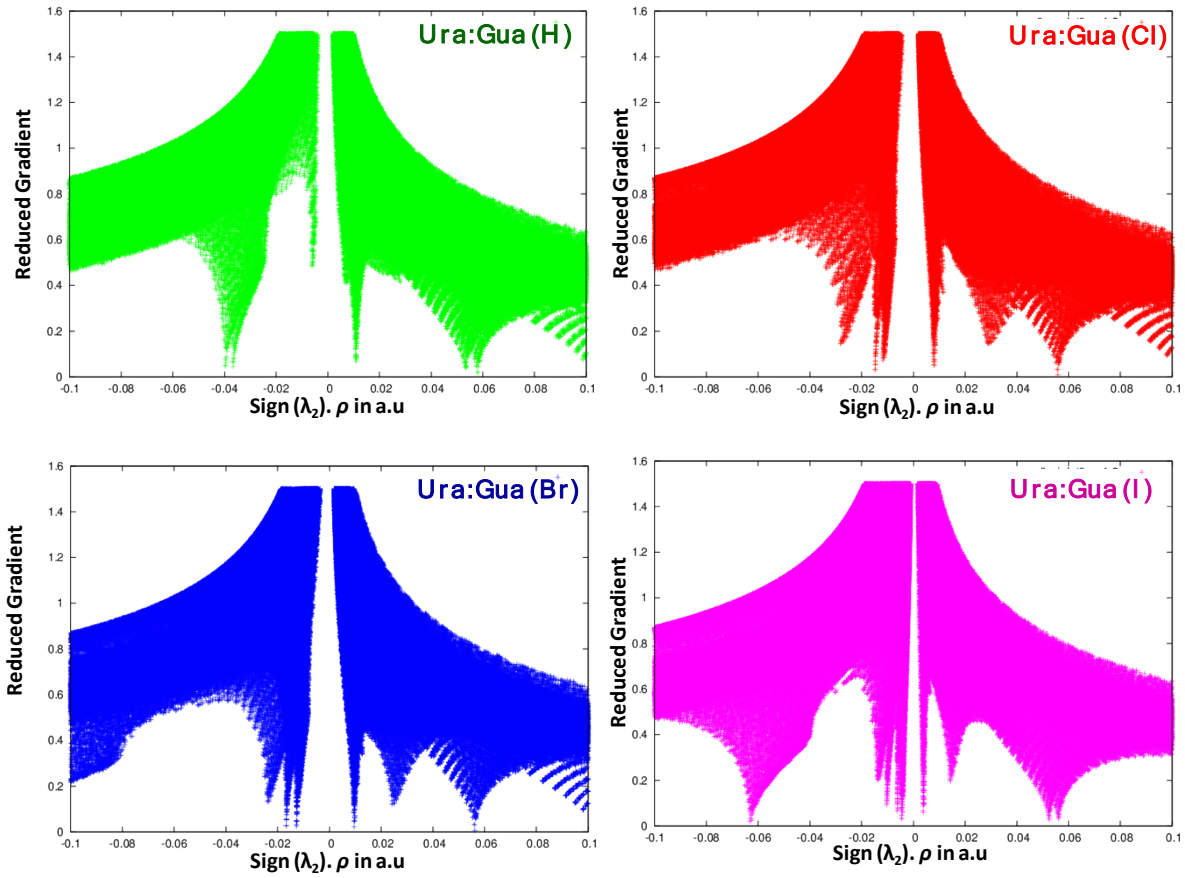
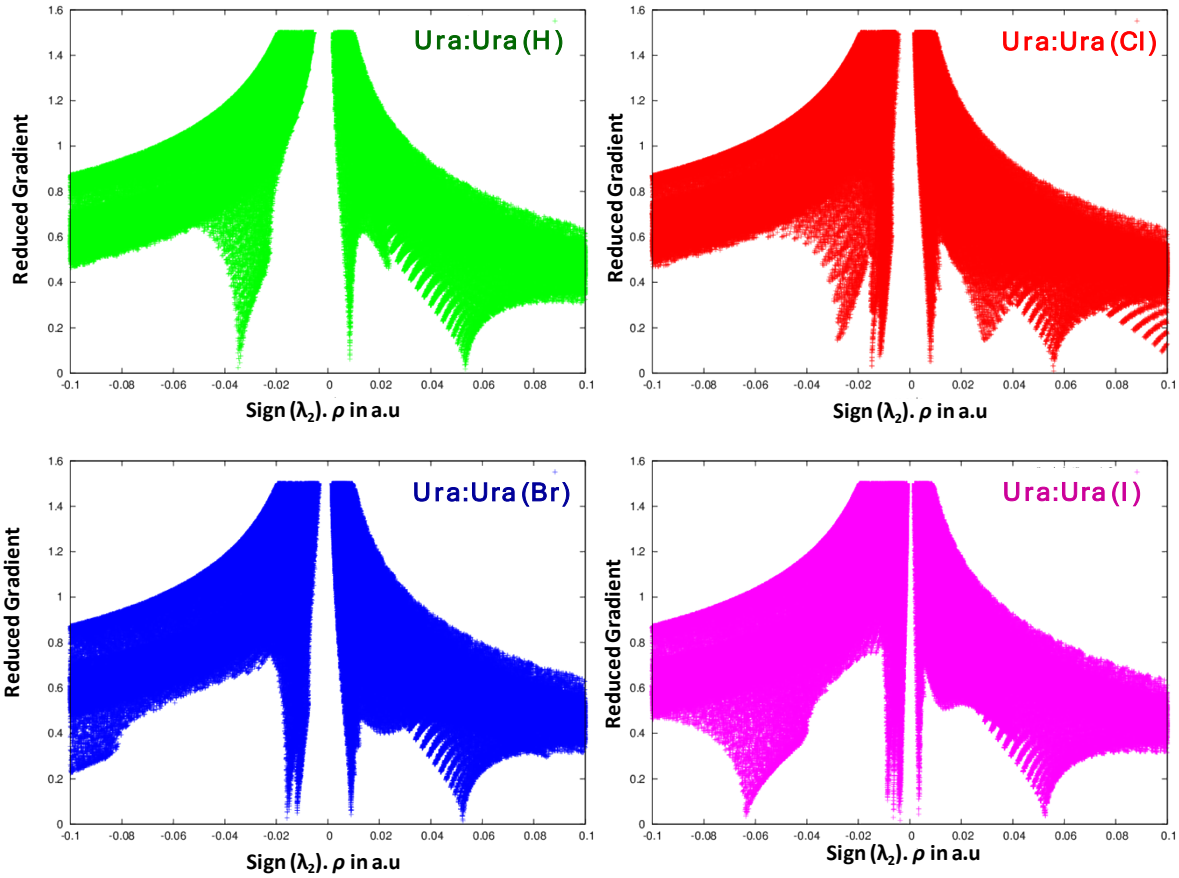
Figure SIF9 The graph of the reduced electron density gradient vs sign of λ_2 in Ura:Gua(X) where X= H, Cl, Br & I