A combined experimental and computational (DFT, RDF, MC and MD) investigation of epoxy resin as a potential corrosion inhibition for mild steel in 0.5 M H_2SO4 environment

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Supporting information

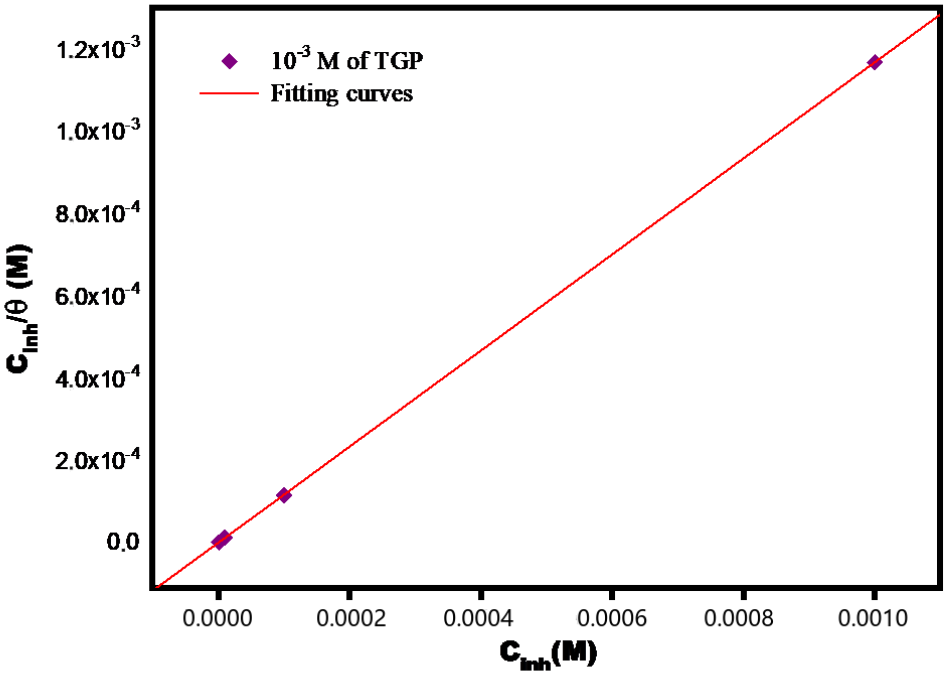

Figure. S1. Langmuir adsorption isotherm model of TGP for MS in 0.5 M H_2SO_4 at 298 K

Table S1. Hirshfeld charges, condensed Fukui functions and condensed dual descriptors for the neutral form of the TGP inhibitor molecules as obtained at the B3LYP/6-31G(d,p)/H_2O/PCM model of theory. Units used below are "e" (elementary charge)

atoms	q_N	q_{N+1}	q_{N-1}	f_k^+	f_k^-	f_k^2	s_k^+	s_k^-	Δs_k	w_k^+	w_k^+	Δw_k
C1	0.1513	-0.1433	0.1993	0.2945	0.0480	0.2465	0.1084	0.0177	0.0907	0.9716	0.1584	0.8132
C2	0.0502	0.0090	0.0776	0.0412	0.0274	0.0138	0.0152	0.0101	0.0051	0.1359	0.0904	0.0455
C3	0.0552	0.0478	0.0757	0.0074	-0.0205	0.0131	0.0027	-0.0075	0.0048	0.0244	-0.0676	0.0432
C4	0.0511	0.0463	0.0738	0.0049	-0.0227	0.0178	0.0018	-0.0084	0.0066	0.0162	-0.0749	0.0587
C5	0.0180	0.0151	0.0439	0.0028	-0.0259	0.0231	0.0010	-0.0095	0.0085	0.0092	-0.0854	0.0762
C6	0.0283	0.0270	0.0401	0.0012	-0.0118	0.0106	0.0004	-0.0043	0.0039	0.0040	-0.0389	0.0350
C7	0.0363	0.0360	0.0393	0.0003	-0.0030	0.0027	0.0001	-0.0011	0.0010	0.0009	-0.0099	0.0089
C8	0.0123	0.0119	0.0164	0.0004	-0.0041	0.0037	0.0001	-0.0015	0.0014	0.0013	-0.0135	0.0122
C9	0.0331	0.0184	0.0471	0.0147	0.0140	0.0007	0.0054	0.0051	0.0003	0.0485	0.0462	0.0023
C10	0.0374	0.0309	0.0404	0.0065	0.0030	0.0035	0.0024	0.0011	0.0013	0.0214	0.0099	0.0115
C11	0.0174	0.0100	0.0239	0.0074	0.0065	0.0009	0.0027	0.0024	0.0003	0.0244	0.0214	0.0030
C12	0.0216	0.0192	0.0439	0.0024	-0.0175	0.0199	0.0009	-0.0064	0.0073	0.0079	-0.0578	0.0657
C13	0.0339	0.0327	0.0387	0.0012	-0.0025	0.0037	0.0004	-0.0010	0.0014	0.0040	-0.0082	0.0122
C14	0.0104	0.0093	0.0179	0.0011	-0.0052	0.0063	0.0004	-0.0019	0.0023	0.0036	-0.0172	0.0208
C15	0.0279	0.0223	0.0420	0.0056	-0.0029	0.0085	0.0020	-0.0011	0.0031	0.0184	-0.0096	0.0280
C16	0.0356	0.0334	0.0391	0.0022	-0.0018	0.0040	0.0008	-0.0007	0.0015	0.0072	-0.0060	0.0132
C17	0.0121	0.0093	0.0178	0.0028	-0.0007	0.0035	0.0010	-0.0002	0.0012	0.0092	-0.0022	0.0114
O18	-0.2482	-0.4921	-0.1539	0.2439	0.0942	0.1497	0.0894	0.0346	0.0548	0.8046	0.3108	0.4938
O19	-0.1591	-0.1951	-0.1033	0.0360	0.0558	0.0198	0.0132	0.0205	0.0073	0.1188	0.1843	0.0655
O20	-0.1594	-0.1649	-0.0916	0.0055	0.0678	0.0623	0.0020	0.0249	0.0229	0.0180	0.2232	0.2052
O21	-0.1726	-0.1753	-0.0772	0.0027	0.0953	0.0928	0.0010	0.0351	0.0341	0.0088	0.3144	0.3056
O22	-0.1647	-0.1666	-0.1250	0.0019	0.0396	0.0377	0.0007	0.0146	0.0139	0.0062	0.1306	0.1244
O23	-0.2252	-0.2365	-0.2183	0.0113	0.0069	0.0044	0.0042	0.0026	0.0016	0.0372	0.0227	0.0145
O24	-0.2256	-0.2275	-0.2144	0.0019	0.0114	0.0095	0.0007	0.0042	0.0035	0.0062	0.0375	0.0313
O25	-0.2243	-0.2251	-0.2168	0.0008	0.0075	0.0067	0.0003	0.0028	0.0025	0.0026	0.0247	0.0221
O26	-0.2229	-0.2269	-0.2138	0.0039	0.0091	0.0052	0.0014	0.0033	0.0019	0.0129	0.0301	0.0172

Table S2. Hirshfeld charges, condensed Fukui functions and condensed dual descriptors for the protonated form of the TGP inhibitor molecules as obtained at the B3LYP/6-31G(d,p)/H_2O/PCM model of theory. Units used below are "e" (elementary charge)

atoms	q_N	q_{N+1}	q_{N-1}	f_k^+	f_k^-	f_k^2	s_k^+	s_k^-	Δs_k	w_k^+	w_k^+	Δw_k
				0.2956	0.0487		0.1082	0.0178		0.3522	0.0580	
C1	0.1478	0.1478	0.1965			0.2469			0.0904			0.2941
				0.0418	0.0267		0.0153	0.0098		0.0498	0.0318	
C2	0.0511	0.0093	0.0778			0.0151			0.0055			0.0180
				0.0058	0.0206		0.0021	0.0075		0.0069	0.0245	
C3	0.0509	0.0450	0.0714			0.0148			0.0054			0.0176
				0.0041	0.0226		0.0015	0.0083		0.0049	0.0269	
C4	0.0470	0.0429	0.0696			0.0185			0.0068			0.0220
				0.0024	0.0196		0.0009	0.0072		0.0029	0.0233	
C5	0.0169	0.0144	0.0365			0.0172			0.0063			0.0205
				0.0022	0.0216		0.0008	0.0079		0.0026	0.0257	
C6	0.0148	0.0126	0.0361			0.0190			0.0070			0.0226
				0.0004	0.0052		0.0001	0.0019		0.0012	0.0062	
C7	0.0500	0.0492	0.0555			0.0047			0.0017			0.0056
				0.0004	0.0041		0.0001	0.0015		0.0005	0.0049	
C8	0.0248	0.0242	0.0289			0.0035			0.0013			0.0042
				0.0143	0.0120		0.0053	0.0044		0.0170	0.0143	
C9	0.0309	0.0166	0.0429			0.0023			0.0008			0.0027
				0.0053	0.0031		0.0020	0.0011		0.0063	0.0037	
C10	0.0473	0.0414	0.0508			0.0024			0.0009			0.0029
				0.0031	0.0025		0.0011	0.0009		0.0037	0.0030	
C11	0.0283	0.0249	0.0310			0.0006			0.0002			0.0007
				0.0010	0.0104		0.0004	0.0038		0.0012	0.0124	
C12	0.0193	0.0181	0.0302			0.0097			0.0036			0.0116
				0.0003	0.0021		0.0001	0.0008		0.0004	0.0025	
C13	0.0504	0.0499	0.0533			0.0025			0.0009			0.0030
				0.0003	0.0024		0.0001	0.0009		0.0004	0.0028	
C14	0.0234	0.0231	0.0260			0.0023			0.0008			0.0027
				0.0035	0.0141		0.0013	0.0052		0.0042	0.0169	
C15	0.0189	0.0141	0.0335			0.0098			0.0036			0.0117
				0.0008	0.0037		0.0003	0.0014		0.0010	0.0044	
C16	0.0522	0.0503	0.0567			0.0026			0.0010			0.0031
				0.0010	0.0021		0.0004	0.0008		0.0012	0.0025	
C17	0.0185	0.0175	0.0209			0.0014			0.0005			0.0017
				0.2484	0.0995		0.0914	0.0366		0.2965	0.1188	
O18	-0.2585	-0.5071	-0.1590			0.1490			0.0545			0.1775
				0.0380	0.0523		0.0140	0.0192		0.0455	0.0626	
O19	-0.1572	-0.1961	-0.1051			0.0132			0.0048			0.0157
				0.0044	0.0662		0.0016	0.0244		0.0053	0.0793	
O20	-0.1599	-0.1641	-0.0932			0.0625			0.0229			0.0745
				0.0024	0.0410		0.0009	0.0151		0.0029	0.0491	
O21	-0.1694	-0.1718	-0.1282			0.0388			0.0142			0.0462
				0.0031	0.0834		0.0011	0.0307		0.0037	0.0999	
O22	-0.1678	-0.1713	-0.0849			0.0795			0.0291			0.0947
				0.0076	0.0048		0.0028	0.0018		0.0091	0.0057	
O23	-0.2596	-0.2677	-0.2539			0.0023			0.0008			0.0027
				0.0004	0.0021		0.0001	0.0008		0.0005	0.0025	
O24	-0.2440	-0.2441	-0.2418			0.0020			0.0007			0.0024
				0.0004	0.0021		0.0001	0.0008		0.0005	0.0025	
O25	-0.2491	-0.2493	-0.2464			0.0024			0.0009			0.0029
				0.0010	0.0031		0.0004	0.0011		0.0012	0.0037	
O26	-0.2421	-0.2431	-0.2390			0.0022			0.0008			0.0026
				0.0031	0.0031		0.0011	0.0011		0.0037	0.0037	
O27	-0.2315	-0.2347	-0.2285			0.0001			0.0000			0.0001
				0.0004	0.0041		0.0001	0.0015		0.0005	0.0049	
O28	-0.2444	-0.2448	-0.2397			0.0043			0.0016			0.0051
				0.0004	0.0114		0.0001	0.0042		0.0005	0.0136	
O29	-0.2559	-0.2564	-0.2445			0.0110			0.0040			0.0131
				0.0031	0.0093		0.0011	0.0034		0.0037	0.0112	
O30	-0.2490	-0.2525	-0.2391			0.0064			0.0023			0.0076