Electrochemical and computational insights on the application of expired Metformin drug as a novel inhibitor for the Sweet corrosion of C1018 steel

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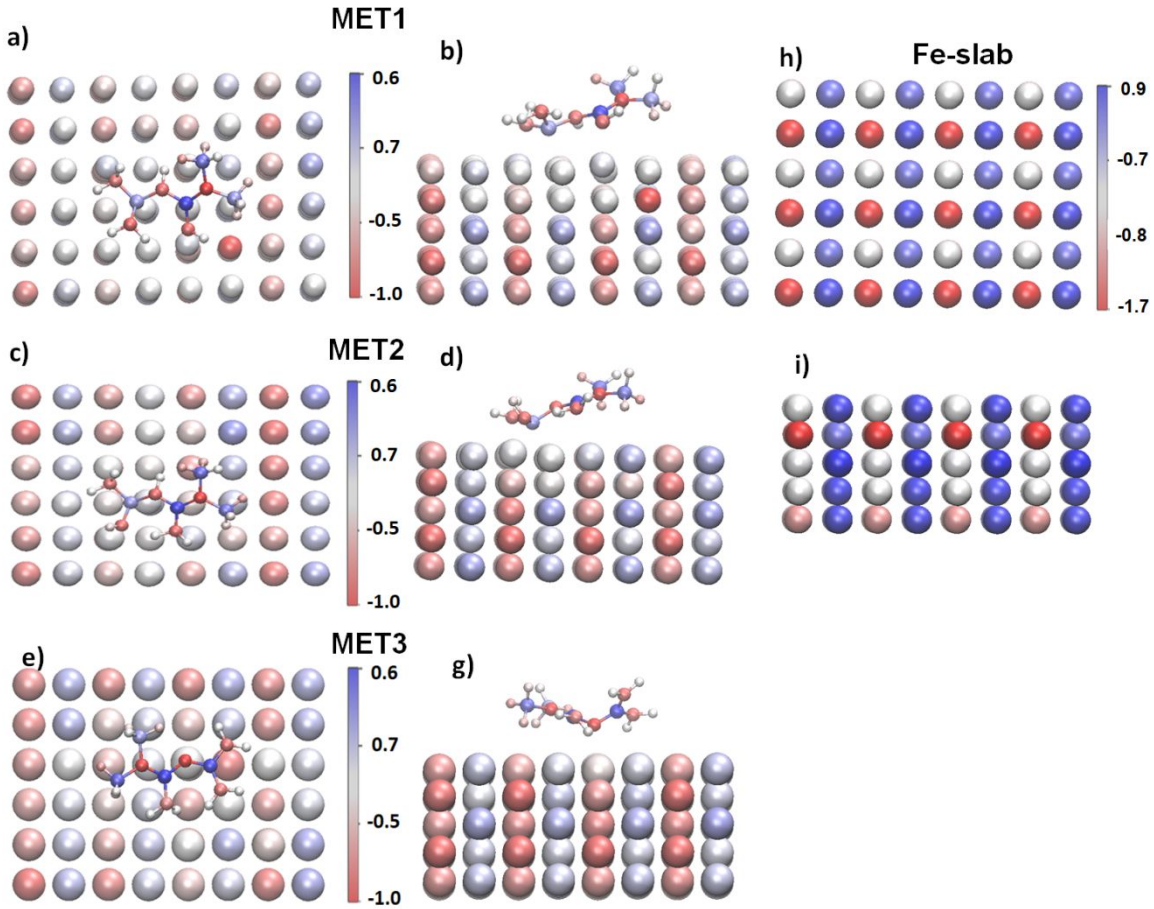

Figure S1 Molecular models of Fe-slab@adsorbate top and side view; MET1 (a & b), MET2 (c & d), MET3 (e & g), and clean slab (h & i). Metformin tautomers are shown in balls and sticks, while slab atoms are shown in spheres. All models are colored based on the atomic charges.

Table S1 Atomic charges calculated using Bader analysis as implemented by Henkelman group.

Atom	MET1	MET2	MET3-I	Fe-slab-clean
Fe	-0.168	-0.379	-0.385	-0.286
Fe	+0.330	+0.317	+0.449	+0.713
Fe	-0.422	-0.328	-0.447	-0.217
Fe	+0.534	+0.529	+0.598	+0.871
Fe	-0.386	-0.423	-0.421	-1.027
Fe	+0.483	+0.531	+0.478	+0.677
Fe	-0.517	-0.529	-0.651	-1.613
Fe	+0.237	+0.332	+0.380	+0.500
Fe	-0.584	-0.576	-0.585	-0.349
Fe	+0.319	+0.385	+0.409	+0.765
Fe	+0.103	+0.243	-0.297	-0.286
Fe	+0.078	+0.222	+0.338	+0.713
Fe	-0.341	-0.518	-0.466	-0.217
Fe	+0.529	+0.551	+0.514	+0.871
Fe	-0.352	-0.444	-0.433	-1.028
Fe	+0.479	+0.437	+0.435	+0.677
Fe	-0.135	-0.210	-0.505	-1.613
Fe	+0.050	-0.017	+0.391	+0.500

Fe	-0.574	-0.571	-0.585	-0.349
Fe	+0.337	+0.335	+0.429	+0.765
Fe	+0.287	+0.327	+0.004	-0.286
Fe	+0.235	+0.458	+0.323	+0.713
Fe	-0.340	-0.364	-0.558	-0.217
Fe	+0.586	+0.561	+0.548	+0.871
Fe	-0.411	-0.399	-0.392	-1.027
Fe	+0.460	+0.495	+0.460	+0.677
Fe	+0.051	-0.304	-0.208	-1.613
Fe	-0.774	-0.152	+0.492	+0.500
Fe	-0.586	-0.564	-0.595	-0.349
Fe	+0.152	+0.293	+0.411	+0.765
Fe	-0.201	-0.295	-0.130	-0.286
Fe	+0.158	+0.513	+0.535	+0.713
Fe	-0.218	-0.315	-0.474	-0.217
Fe	+0.540	+0.550	+0.556	+0.871
Fe	-0.281	-0.373	-0.447	-1.027
Fe	+0.449	+0.438	+0.452	+0.677
Fe	-0.310	-0.529	-0.562	-1.613
Fe	+0.341	+0.439	+0.545	+0.500
Fe	-0.565	-0.586	-0.575	-0.349
Fe	+0.339	+0.363	+0.420	+0.765
Fe	-0.242	-0.209	-0.389	-0.286
Fe	+0.023	+0.243	+0.284	+0.713
Fe	-0.330	-0.385	-0.350	-0.217
Fe	+0.452	+0.451	+0.518	+0.870
Fe	-0.387	-0.363	-0.404	-1.027
Fe	+0.406	+0.485	+0.483	+0.677
Fe	-0.340	-0.272	-0.366	-1.613
Fe	+0.057	+0.354	+0.211	+0.502
Fe	-0.507	-0.587	-0.533	-0.350
Fe	+0.328	+0.348	+0.343	+0.765
Fe	+0.357	+0.039	-0.242	-0.287
Fe	+0.231	+0.268	+0.314	+0.713
Fe	-0.398	-0.447	-0.372	-0.217
Fe	+0.406	+0.497	+0.496	+0.870
Fe	-0.438	-0.418	-0.403	-1.027
Fe	+0.442	+0.406	+0.440	+0.677
Fe	-0.025	-0.043	-0.144	-1.613
Fe	+0.264	-0.036	+0.260	+0.502
Fe	-0.496	-0.554	-0.538	-0.349
Fe	+0.344	+0.342	+0.339	+0.765
Fe	+0.097	-0.340	+0.116	-0.287
Fe	+0.203	+0.374	+0.092	+0.713
Fe	-0.341	-0.337	-0.287	-0.217
Fe	+0.597	+0.520	+0.529	+0.870
Fe	-0.351	-0.347	-0.375	-1.027
Fe	+0.402	+0.476	+0.472	+0.677
Fe	-0.008	-0.102	-0.341	-1.613
Fe	+0.371	+0.424	-0.560	+0.501
Fe	-0.486	-0.580	-0.519	-0.350
Fe	+0.360	+0.337	+0.211	+0.765
Fe	-0.233	-0.481	+0.006	-0.286
Fe	+0.415	+0.385	+0.277	+0.713
Fe	-0.342	-0.398	-0.243	-0.217
Fe	+0.473	+0.546	+0.494	+0.870
Fe	-0.422	-0.428	-0.304	-1.027
Fe	+0.479	+0.446	+0.429	+0.677
Fe	-0.441	-0.494	-0.375	-1.612
Fe	+0.596	+0.492	+0.299	+0.501
Fe	-0.485	-0.595	-0.521	-0.350
Fe	+0.340	+0.338	+0.351	+0.765
Fe	-0.384	-0.544	-0.465	-0.287
Fe	+0.211	+0.487	+0.474	+0.713
Fe	-0.500	-0.484	-0.422	-0.216
Fe	+0.522	+0.525	+0.539	+0.871
Fe	-0.453	-0.431	-0.434	-1.029
Fe	+0.471	+0.501	+0.452	+0.678
Fe	-0.540	-0.611	-0.505	-1.613
Fe	+0.395	+0.468	+0.508	+0.501
Fe	-0.547	-0.602	-0.568	-0.352
Fe	+0.400	+0.427	+0.405	+0.766

Fe	-0.106	-0.312	-0.466	-0.287
Fe	-0.134	+0.178	+0.310	+0.713
Fe	-0.502	-0.480	-0.468	-0.216
Fe	+0.484	+0.473	+0.455	+0.871
Fe	-0.414	-0.390	-0.425	-1.029
Fe	+0.432	+0.420	+0.427	+0.678
Fe	-0.355	-0.369	-0.161	-1.613
Fe	+0.261	+0.253	+0.441	+0.501
Fe	-0.503	-0.549	-0.562	-0.352
Fe	+0.419	+0.402	+0.443	+0.766
Fe	-0.039	-0.385	-0.484	-0.287
Fe	+0.101	+0.623	+0.371	+0.713
Fe	-0.443	-0.440	-0.456	-0.216
Fe	+0.446	+0.537	+0.590	+0.871
Fe	-0.419	-0.424	-0.479	-1.029
Fe	+0.474	+0.483	+0.490	+0.678
Fe	-0.232	-0.128	-0.239	-1.613
Fe	+0.389	+0.502	+0.517	+0.501
Fe	-0.488	-0.571	-0.553	-0.352
Fe	+0.413	+0.440	+0.425	+0.766
Fe	-0.123	-0.528	-0.457	-0.287
Fe	+0.463	+0.556	+0.440	+0.713
Fe	-0.477	-0.512	-0.479	-0.216
Fe	+0.494	+0.526	+0.544	+0.871
Fe	-0.474	-0.438	-0.455	-1.028
Fe	+0.422	+0.438	+0.468	+0.678
Fe	-0.547	-0.603	-0.452	-1.613
Fe	+0.463	+0.665	+0.490	+0.501
Fe	-0.519	-0.556	-0.600	-0.352
Fe	+0.425	+0.414	+0.436	+0.766
N	-0.567	-0.617	-0.646	NA
N	-0.670	-0.635	-0.607	NA
N	-0.640	-0.673	-0.952	NA
N	-0.654	-0.651	-0.520	NA
N	-0.882	-0.865	-0.866	NA
H	+0.174	+0.117	+0.126	NA
H	-0.021	+0.211	+0.174	NA
H	+0.119	-0.112	+0.105	NA
H	+0.058	+0.010	+0.206	NA
H	-0.034	+0.143	+0.192	NA
H	+0.089	+0.150	-0.010	NA
H	-0.410	-0.366	-0.061	NA
H	+0.046	+0.033	-0.471	NA
H	-0.196	-0.315	-0.173	NA
H	-0.025	-0.078	-0.254	NA
H	-0.199	-0.148	-0.180	NA
H	-0.217	-0.398	-0.033	NA
C	+0.653	+0.667	+1.057	NA
C	+1.127	+1.094	+1.135	NA
C	+0.823	+0.868	+0.914	NA
C	+0.655	+0.807	+0.622	NA