Electronic Supplementary Information for:

Structure Determination of the Oxygen Evolution Catalyst Mössbauerite

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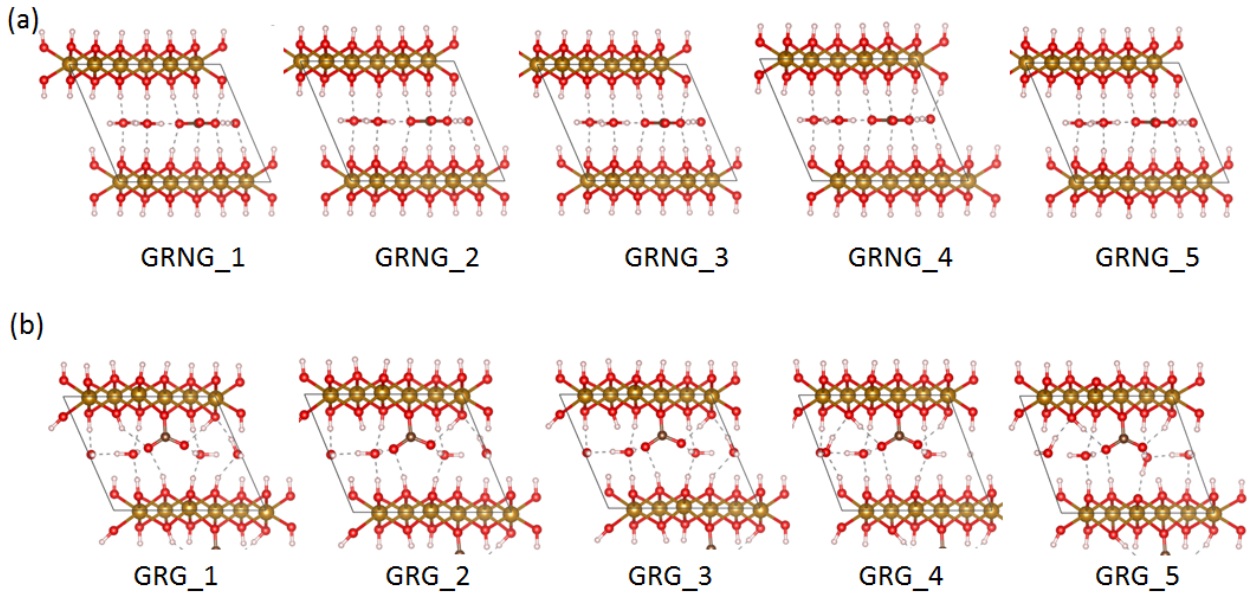

Figure S1: The side views of optimized lowest energy structures for green rust with carbonate (a) non-grafted (GRNG_1 to GRNG_5) and (b) grafted (GRG_1 to GRG_5).

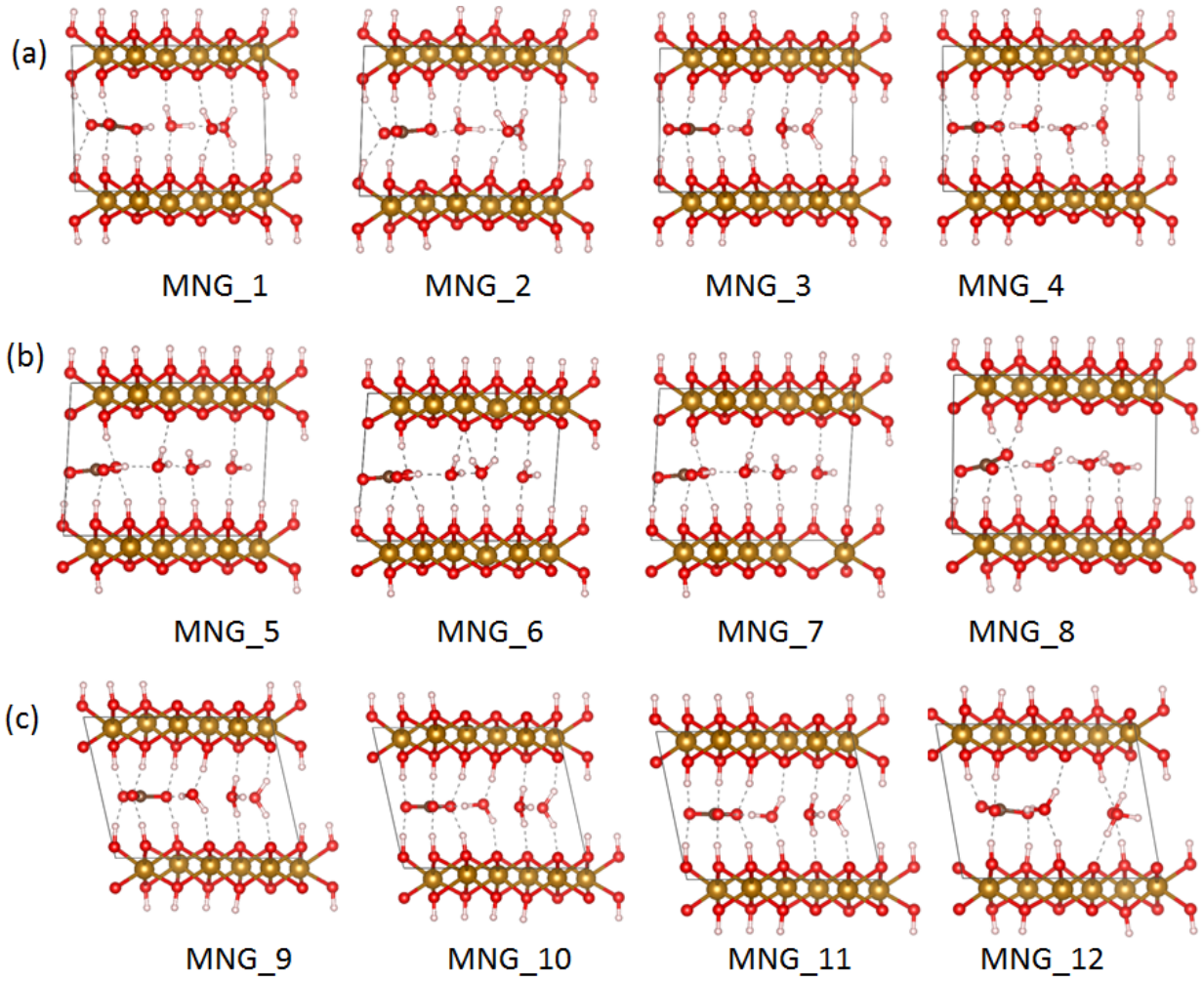

Figure S2: The side views of optimized lowest energy structures for mössbauerite with carbonate non-grafted for (a) ($5OH^-/3OH^-$) configuration from MNG_1 to MNG_4, (b) ($6OH^-/2OH^-$) configuration from MNG_5 to MNG_8, and (c) ($4OH^-/4OH^-$) configuration from MNG_9 to MNG_12.

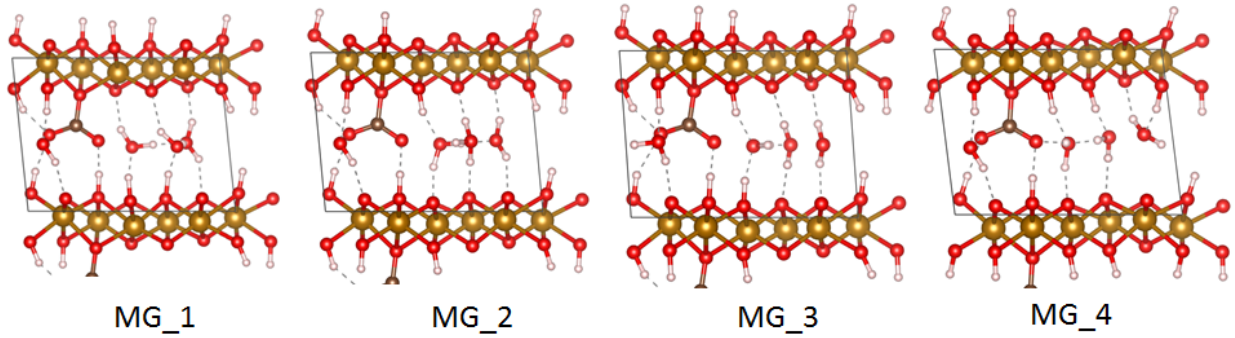

Figure S3: The side views of optimized lowest energy structures for mössbauerite with carbonate grafted for ($5OH^-/2OH^-$) configuration from MG_1 to MG_4.

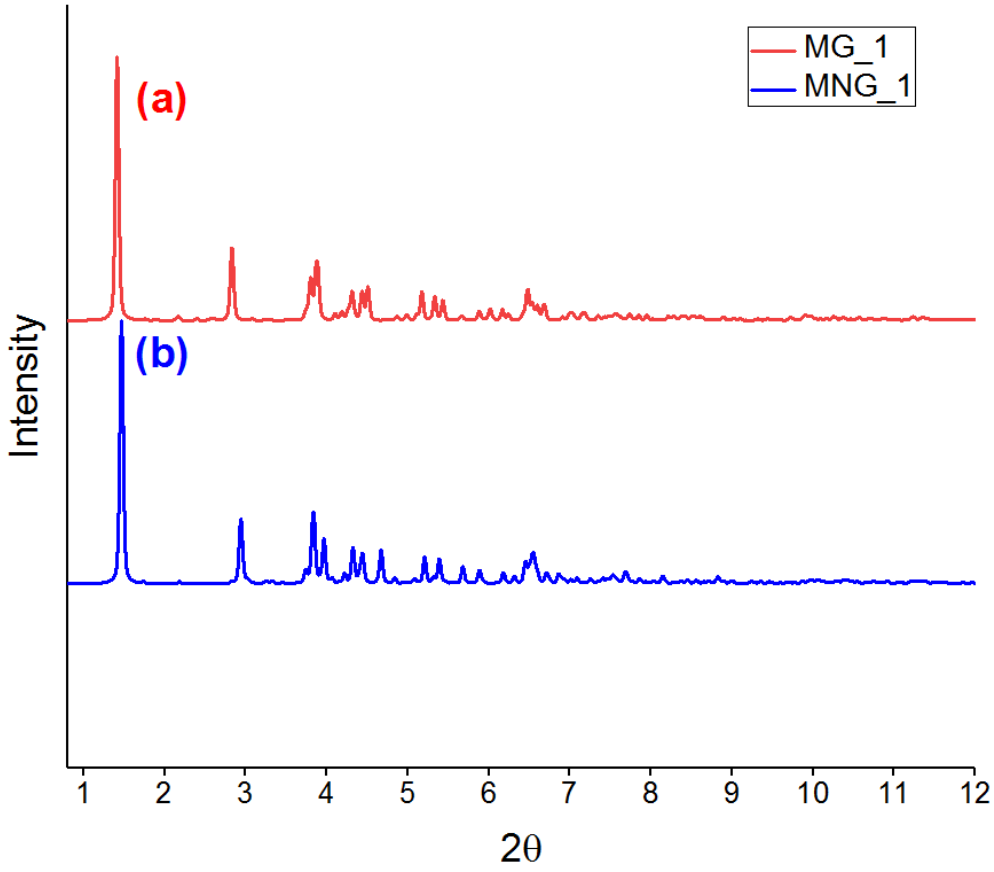

Figure S4: Simulated PXRD patterns for mössbauerite structure (a) without grafting ($5OH^-/3OH^-$)-MNG_1 and (b) with grafting ($5OH^-/2OH^-$)-MG_1 of carbonate.

S5: Cif file for computational geometry optimized structure for non-grafted mössbauerite [($5OH^-/3OH^-$)-MNG_1 in Tab. 2].

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CRYSTAL DATA

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H5	1.0	0.759312	0.669644	0.230117	Biso	1.000000	H
H6	1.0	0.168896	0.486289	0.570996	Biso	1.000000	H
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H8	1.0	0.501039	0.837720	0.556074	Biso	1.000000	H
H9	1.0	0.410140	0.828974	0.322929	Biso	1.000000	H
H10	1.0	0.709403	0.752129	0.439122	Biso	1.000000	H
H11	1.0	0.882710	0.679442	0.549279	Biso	1.000000	H
H12	1.0	0.879192	0.154353	0.662042	Biso	1.000000	H
H13	1.0	0.746975	0.402633	0.440690	Biso	1.000000	H
H14	1.0	0.252447	0.008374	0.655860	Biso	1.000000	H
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Fe5	1.0	0.982060	0.816508	0.935824	Biso	1.000000	Fe
Fe6	1.0	0.651311	0.981748	0.955177	Biso	1.000000	Fe
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O9	1.0	0.281829	0.993826	0.795082	Biso	1.000000 O
O10	1.0	0.693863	0.156298	0.092771	Biso	1.000000 O
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O17	1.0	0.450059	0.783357	0.439825	Biso	1.000000 O
O18	1.0	0.854047	0.722976	0.428389	Biso	1.000000 O

S6: Cif file for computational geometry optimized structures for grafted mössbauerite [($5OH^-/3OH^-$)-MG_1 in Tab. 2].

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CRYSTAL DATA

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H7	1.0	0.261912	0.635344	0.434834	Biso	1.000000	H
H8	1.0	0.556283	0.835128	0.579885	Biso	1.000000	H
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H11	1.0	0.919484	0.680718	0.516854	Biso	1.000000	H
H12	1.0	0.890892	0.140111	0.652684	Biso	1.000000	H
H13	1.0	0.562698	0.109669	0.444969	Biso	1.000000	H
H14	1.0	0.247628	0.026011	0.664348	Biso	1.000000	H
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O3	1.0	0.612590	0.831837	0.810713	Biso	1.000000	O
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O9	1.0	0.261265	-0.006117	0.798801	Biso	1.000000	O
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O11	1.0	0.386406	0.345464	0.090230	Biso	1.000000	O
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O13	1.0	0.366910	0.845274	0.082284	Biso	1.000000	O
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O15	1.0	0.063257	0.023818	0.115970	Biso	1.000000	O
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O18	1.0	0.930119	0.750387	0.421432	Biso	1.000000	O