Table S1. Coordinates of the optimized structure and Mulliken charges for partially hydrated MgO (model A in Figure 3).

		Coordinates			Mulliken
	Atoms	x	y	z	charges
1	Mg	-2.00809	-0.87562	-1.82088	0.88456
2	O	-1.97383	-1.03026	0.146515	-0.88239
3	Mg	-1.58096	-0.90643	2.0417	0.894351
4	O	-0.76204	0.850771	2.0513	-0.89502
5	Mg	0.495138	2.315759	1.804889	0.857988
6	Mg	1.093031	-0.32738	1.898459	0.902687
7	Mg	-0.21678	-2.24411	-0.33707	0.743281
8	Mg	-0.92332	0.783637	0.033942	0.996994
9	O	0.205845	2.546319	-0.08189	-0.88972
10	O	2.135439	1.317523	1.714503	-0.85914
11	O	0.017953	-1.78366	2.70086	-0.87909
12	O	-0.48291	-1.93297	-2.25949	-0.86916
13	O	-1.20235	0.878111	-1.97979	-0.88399
14	Mg	1.947236	1.250592	-0.25408	0.88314
15	Mg	0.6532	-0.35619	-2.18159	0.910087
16	Mg	0.106856	2.310572	-1.98854	0.869999
17	O	0.849471	-0.49333	-0.10925	-0.91750
18	O	1.716785	1.284653	-2.21916	-0.86164
19	H	0.154028	-2.68015	2.285503	0.48027
20	O	0.086634	-3.65693	0.870182	-0.88401
21	H	0.32220	-4.57158	0.682291	0.398292

Table S2. Coordinates of the optimized structure, Mulliken charges and spin densities for MgO with stabilized O^{-}_{3C} (model B in Figure 3).

		Coordinates			Mulliken	Spin
	Atoms	x	y	z	charges	densities
1	Mg	-2.04483	-0.79369	-1.90124	0.855355	-0.00047
2	O	-1.94342	-1.07612	0.031478	-0.88714	0.001141
3	Mg	-1.23129	-1.46854	1.876655	0.877817	-0.02911
4	O	-0.61534	0.468853	2.095626	-0.8635	0.056273
5	Mg	0.470478	2.094785	1.964818	0.848689	-0.00752
6	Mg	1.297638	-0.4244	1.814336	0.847782	-0.0173
7	Mg	-0.23638	-2.20086	-0.56086	0.873192	-0.00221
8	Mg	-0.98952	0.693003	0.126136	0.974748	0.003544
9	O	0.069507	2.483016	0.1238	-0.88963	0.002427
10	O	2.20094	1.28906	1.696877	-0.86554	-0.00067
11	O	0.465549	-1.81246	2.967428	-0.49473	0.946469
12	O	-0.48596	-1.79138	-2.44006	-0.86438	0.000057
13	O	-1.25742	0.961394	-1.91945	-0.88972	0.000053
14	Mg	1.905366	1.317726	-0.23917	0.879868	0.00178
15	Mg	0.601508	-0.17454	-2.24128	0.878426	-0.00017
16	Mg	-0.0365	2.443521	-1.79659	0.882897	0.000043

17	O	0.939592	-0.55778	-0.19227	-0.88668	0.000669
18	O	1.604853	1.506261	-2.1651	-0.86538	0.000225
19	O	-0.58847	-3.23478	1.04037	-0.83278	0.045982
20	H	0.043679	-3.73247	1.576749	0.420708	-0.00123

Table S3. Coordinates of the optimized structure and Mulliken charges for the initial Mg9O9 cluster (model C in Figure 3).

			Coordinates		Mulliken
	Atoms	x	y	z	charges
1	O	-1.89476	-2.07529	1.036505	-0.852
2	Mg	-1.83138	-2.00426	-0.87953	0.847032
3	Mg	0.089658	-1.99842	1.055886	0.883021
4	O	2.072786	-1.89732	1.037236	-0.85183
5	O	0.09269	-2.07032	-1.14036	-0.88155
6	Mg	2.002585	-1.83352	-0.87886	0.84683
7	O	-2.07264	1.897486	1.037205	-0.85198
8	Mg	-2.00235	1.83372	-0.87868	0.847106
9	O	-2.07822	-0.09279	-1.13055	-0.88135
10	Mg	-2.00122	-0.08997	1.04968	0.884752
11	Mg	-0.08975	1.998285	1.055359	0.882846
12	O	1.894275	2.075872	1.036921	-0.85192
13	O	-0.09282	2.068766	-1.14195	-0.88168
14	Mg	1.830282	2.005099	-0.87907	0.846937
15	Mg	-0.00014	-0.00083	-1.12682	0.969225
16	O	0.000244	0.000011	1.046328	-0.9589
17	O	2.078468	0.093118	-1.13008	-0.88138
18	Mg	2.002294	0.090212	1.047862	0.884829

Table S4. Coordinates of the optimized structure, Mulliken charges and spin densities for MgO with stabilized hydrogen atom (model D in Figure 3).

			Coordinates		Mulliken	Spin
	Atoms	x	y	z	charges	densities
1	O	2.026206	1.984266	0.999568	-0.84965	0.001231
2	Mg	1.926322	1.927609	-0.91564	0.857693	0.010086
3	Mg	0.040334	1.999684	1.029359	0.799425	0.122985
4	O	-1.96808	1.8989	1.090116	-0.85201	0.002452
5	O	-0.02772	2.040209	-1.08454	-0.88875	0.004336
6	Mg	-1.9821	2.005094	-0.8359	0.772661	0.228296
7	O	2.026427	-1.98404	0.999571	-0.84965	0.00123
8	Mg	1.926537	-1.92739	-0.91564	0.85769	0.010085
9	O	2.071295	0.000119	-1.17368	-0.87775	-0.00081
10	Mg	2.051828	0.000116	1.027627	0.845839	0.035352
11	Mg	0.040561	-1.99969	1.029353	0.799438	0.122972
12	O	-1.96787	-1.89912	1.090105	-0.85201	0.002451
13	O	-0.0275	-2.04023	-1.08454	-0.88875	0.004335
14	Mg	-1.98186	-2.00529	-0.8359	0.772702	0.228235
15	Mg	0.028446	0	-1.13991	0.886696	0.117781

16	O	0.037905	0	1.086941	-0.95356	-0.00084
17	O	-2.08946	-0.00013	-1.47416	-0.83606	-0.01293
18	Mg	-1.90169	-0.00011	1.456097	0.829296	0.099688
19	H	-2.43031	-0.00012	-2.38837	0.426742	0.023071