

Supplementary material

Table S1 Adsorption energy of water on malachite ($\bar{2}01$) surface

Site	E_{ini}/eV	E_{fin}/eV	E_{ads}/eV
1	-715.137	-715.212	-0.08
2	-715.137	-715.371	-0.23
3	-715.137	-715.313	-0.18
4	-715.137	-715.299	-0.16
5	-715.137	-715.256	-0.12
6	-715.137	-715.235	-0.10
7	-715.137	-715.155	-0.02
8	-715.137	-715.115	0.02

Table S2 Adsorption energy of water on malachite (201) surface

Site	E_{ini}/eV	E_{fin}/eV	E_{ads}/eV
1	-797.493	-798.287	-0.79
2	-797.493	-798.178	-0.69
3	-797.493	-798.385	-0.89
4	-797.493	-798.122	-0.63
5	-797.493	-798.644	-1.151
6	-797.493	-797.920	-0.43
7	-797.493	-797.682	-0.19
8	-797.493	-797.708	-0.21

Table S3 Adsorption energy of water on malachite (010) surface

Site	E_{ini}/eV	E_{fin}/eV	E_{ads}/eV
1	-744.151	-744.585	-0.43
2	-744.151	-738.502	5.65

Table S4 Adsorption energy of water on malachite (001) surface

Site	E_{ini}/eV	E_{fin}/eV	E_{ads}/eV
1	-747.296	-747.872	-0.58
2	-747.296	-747.421	-0.12
3	-747.296	-747.572	-0.28
4	-747.296	-747.826	-0.53

Table S5 Adsorption energy of water on malachite (100) surface

Site	E_{ini}/eV	E_{fin}/eV	E_{ads}/eV
1	-768.018	-768.478	-0.46
2	-768.018	-768.356	-0.34

Table S6 Adsorption energy of water on malachite (110) surface

Site	E_{ini}/eV	E_{fin}/eV	E_{ads}/eV
1	-794.368	-795.247	-0.88
2	-794.368	-795.516	-1.148
3	-794.368	-795.000	-0.63