

Supplementary information

Water adsorption on MgO surfaces: a vibrational analysis

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The following structures have been found by first optimizing the geometry of a slab of MgO made of 4 layers orthogonal to (001), (011) or (112) directions, then adding along the vertical z-direction one(two) molecule(s) of H₂O to their top layer per unit surface, starting at a (HO)H---O(Mg) distance around 2 Å, before reoptimizing the whole systems.

1H₂O/MgO (001)

MG	-1.904152901912E+00	1.202386021469E-01	3.201138260738E+00
MG	1.204015095568E-01	-1.932421409982E+00	3.060863796791E+00
O	1.159910295503E-01	1.145817410893E-01	3.192221263135E+00
O	-1.926316481162E+00	-1.929212018051E+00	3.126347341905E+00
MG	1.251270212404E-01	1.150565857947E-01	1.014745774091E+00
MG	-1.925448159700E+00	-1.929401045121E+00	1.025940910413E+00
O	-1.923982549320E+00	1.158676096850E-01	1.023454482258E+00
O	1.229981329061E-01	-1.930236630690E+00	1.011986361569E+00
MG	-1.924071588752E+00	1.156275168201E-01	-1.083098461592E+00
MG	1.236799082830E-01	-1.929889137999E+00	-1.092270454950E+00
O	1.241603388932E-01	1.157011760497E-01	-1.081708148621E+00
O	-1.924476056465E+00	-1.929953170556E+00	-1.082219135231E+00
MG	1.239833363805E-01	1.157439747447E-01	-3.171896808139E+00
MG	-1.924300716317E+00	-1.930105663901E+00	-3.170673547118E+00
O	-1.924118775344E+00	1.153824394746E-01	-3.237216333654E+00
O	1.239082730244E-01	-1.929829543824E+00	-3.237708678138E+00
H	7.634068929402E-01	5.947582701023E-02	4.892723337785E+00
H	1.764855594586E+00	-8.484359802521E-01	5.673599916758E+00
O	1.627523230280E+00	7.098433046348E-02	5.387127452240E+00

2H₂O/MgO (001)

MG	-1.982654131534E+00	1.215467083197E-01	3.040216494402E+00
MG	2.290227884111E-02	-1.935925402323E+00	3.143927242696E+00
O	4.783251529901E-02	1.126379561380E-01	3.166829591678E+00
O	-2.025977270752E+00	-1.934531897764E+00	3.070108552078E+00
MG	4.443448282780E-02	1.174862873840E-01	9.819486434056E-01
MG	-2.011702074716E+00	-1.937504495584E+00	9.896206363868E-01
O	-2.002054129828E+00	1.153896074899E-01	9.780182574656E-01
O	3.387780556211E-02	-1.935614063868E+00	9.894891079057E-01
MG	-2.005287087596E+00	1.143828729468E-01	-1.123472574416E+00
MG	3.729228693129E-02	-1.934469243541E+00	-1.116531667260E+00

O	3.986522280198E-02	1.186285465960E-01	-1.113580542734E+00
O	-2.008304296686E+00	-1.938750455126E+00	-1.114978312323E+00
MG	3.879546695331E-02	1.188337523868E-01	-3.202400950387E+00
MG	-2.007584588038E+00	-1.939112176819E+00	-3.201645456216E+00
O	-2.006331955061E+00	1.140325489372E-01	-3.268557282424E+00
O	3.829697311035E-02	-1.934137681282E+00	-3.268039103891E+00
H	8.246055911627E-01	5.572485484699E-03	4.783833426559E+00
H	-2.004337790737E+00	-6.986269721100E-01	5.512637544046E+00
O	1.620469030352E+00	1.620038470775E-01	5.377156739376E+00
H	-1.235043165610E+00	1.413257560249E+00	5.332407305397E+00
H	1.072858513590E-01	1.734468521331E+00	6.053477241622E+00
O	-5.447059430917E-01	-1.991071353050E+00	5.439915142823E+00

H₂O/MgO (011)

MG	-1.738668769551E+00	8.828673857682E-01	2.090725566598E+00
MG	-1.775612749862E+00	-1.963329463497E+00	2.339597579032E+00
O	2.348718849224E-01	9.269754507271E-01	2.214771201358E+00
O	2.108313746076E-01	-2.157790331087E+00	2.176591064511E+00
MG	2.217911625352E-01	-7.067241459057E-01	7.762057973000E-01
MG	2.286452342291E-01	2.620010048982E+00	9.040391912722E-01
O	-1.763198188355E+00	-6.108062337446E-01	7.270981894149E-01
O	-1.756114004897E+00	2.463278598502E+00	8.617978234603E-01
MG	-1.760673927871E+00	-2.198304578048E+00	-8.338543639510E-01
MG	-1.761892714799E+00	9.182013563615E-01	-8.187463444889E-01
O	2.243440583821E-01	-2.193697106215E+00	-7.647458523493E-01
O	2.231293994974E-01	9.180094138254E-01	-7.376629976759E-01
MG	2.242522151822E-01	2.482052900394E+00	-2.010290142027E+00
MG	2.239360139696E-01	-6.254951350119E-01	-2.063523420256E+00
O	-1.760654993318E+00	2.484388825536E+00	-2.149078415380E+00
O	-1.761041635612E+00	-6.410753907167E-01	-2.199157957182E+00
H	3.348142677075E-01	4.649519247362E-01	3.073817158020E+00
O	-1.873831802521E+00	-3.708162894907E-01	3.633373150459E+00
H	-1.259621944696E+00	-4.078660596996E-01	4.379042771881E+00

H₂O/MgO (112)

MG	2.138550181007E+00	1.042172223766E+00	2.053171973981E+00
MG	-7.155210031359E-01	1.042114187334E+00	2.053177525789E+00
O	-7.581129870649E-01	-4.483272362240E-01	9.232965662939E-01
O	2.181755426329E+00	-4.482817917245E-01	9.232909064382E-01
MG	7.117583876179E-01	-2.845097120601E-01	-4.801346513736E-01
MG	-2.240774918513E+00	-2.012165450457E-01	-4.303539438189E-01
O	-2.241043487840E+00	2.229965058343E+00	1.625640110598E+00
O	7.114960663864E-01	2.540448726544E+00	1.627887274296E+00
MG	-8.214965184615E-01	-2.356992815508E+00	5.641452094664E-01
MG	2.245283214561E+00	-2.356966757679E+00	5.640514795489E-01
O	2.187873719468E+00	9.598614223969E-01	-1.480420828354E+00
O	-7.645334740169E-01	9.597266710686E-01	-1.480475985536E+00
MG	-2.240900439049E+00	2.116405669076E+00	-1.630612234098E+00
MG	7.116258498775E-01	2.093773711429E+00	-1.683473125177E+00
O	7.119067788561E-01	-2.208049464357E+00	-7.995773692652E-01
O	-2.240587891253E+00	-2.132891994331E+00	-8.319462038170E-01
H	7.119418459012E-01	-2.939386454500E+00	2.507002108597E+00
H	7.116248224738E-01	2.086173920622E-03	4.016666053317E+00
O	7.115967831169E-01	7.921175418091E-01	3.458665133113E+00