

## A first principle study of water adsorbed on flat and stepped silver surfaces

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### Test results of simulation parameters

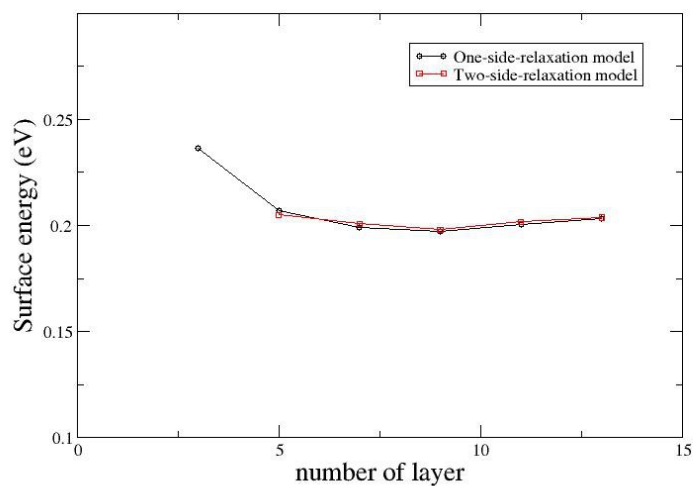


Fig. S1 The surface energy of Ag(100) surface converge with respect to the number of layers with two different slab model.

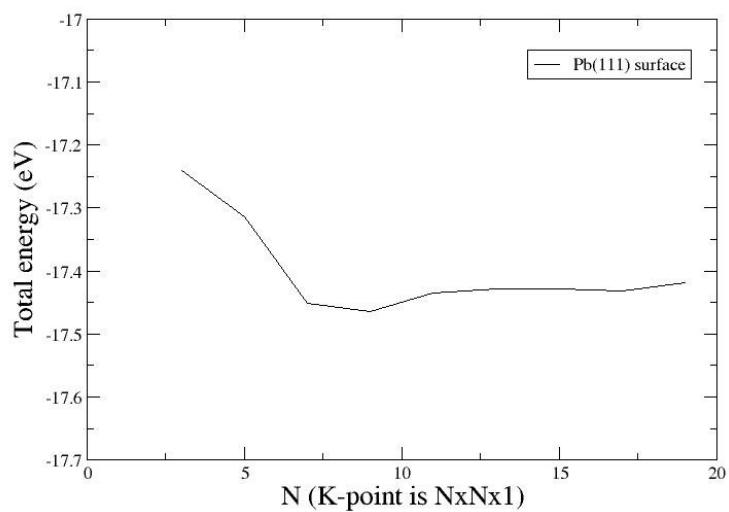


Fig. S2 The total energy of Ag(100) surface converge with respect to the number of K-point

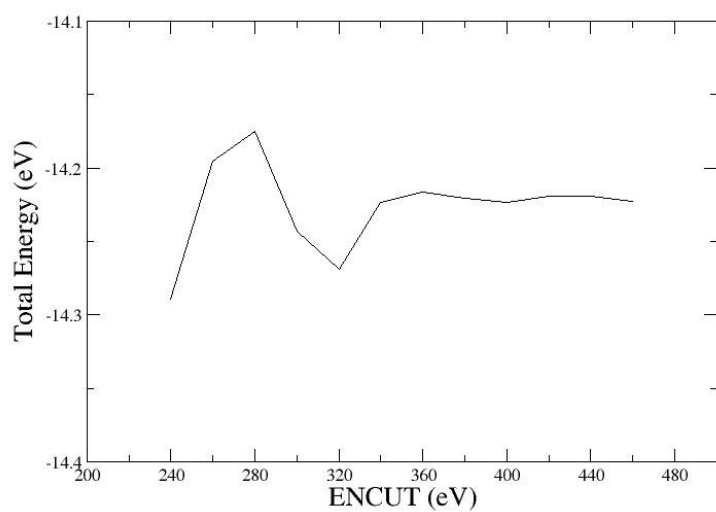


Fig. S3 The total energy of water molecule converge with respect to the value of the Encut

## Structure information

Ag(100) within a 3 x 3 geometry POSCAR

Ag(100)

1.0000000000000000

8.8200000000000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.8200000000000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.3150000000000013

45

Selective dynamics

Direct

0.0572562358276656	0.0000000000000000	0.0000000000000000	F	F	F
0.0572562358276656	0.0000000000000000	0.1468479604449939	F	F	F
0.0572562358276656	0.0000000000000000	0.2932018493337858	T	T	T
0.2239229024943299	0.1666666666666643	0.0734239802224934	F	F	F
0.2239229024943299	0.1666666666666643	0.2208972872956667	T	T	T
0.3905895691609942	0.0000000000000000	0.0000000000000000	F	F	F
0.3905895691609942	0.0000000000000000	0.1468479604449939	F	F	F
0.3905895691609942	0.0000000000000000	0.2932018493337858	T	T	T
0.5572562358276656	0.1666666666666643	0.0734239802224934	F	F	F
0.5572562358276656	0.1666666666666643	0.2208972872956667	T	T	T
0.7239229024943299	0.0000000000000000	0.0000000000000000	F	F	F
0.7239229024943299	0.0000000000000000	0.1468479604449939	F	F	F
0.7239229024943299	0.0000000000000000	0.2932018493337858	T	T	T
0.8905895691609942	0.1666666666666643	0.0734239802224934	F	F	F
0.8905895691609942	0.1666666666666643	0.2208972872956667	T	T	T
0.0572562358276656	0.3333333333333357	0.0000000000000000	F	F	F
0.0572562358276656	0.3333333333333357	0.1468479604449939	F	F	F
0.0572562358276656	0.3333333333333357	0.2932018493337858	T	T	T
0.2239229024943299	0.5000000000000000	0.0734239802224934	F	F	F
0.2239229024943299	0.5000000000000000	0.2208972872956667	T	T	T
0.3905895691609942	0.3333333333333357	0.0000000000000000	F	F	F
0.3905895691609942	0.3333333333333357	0.1468479604449939	F	F	F
0.3905895691609942	0.3333333333333357	0.2932018493337858	T	T	T
0.5572562358276656	0.5000000000000000	0.0734239802224934	F	F	F
0.5572562358276656	0.5000000000000000	0.2208972872956667	T	T	T
0.7239229024943299	0.3333333333333357	0.0000000000000000	F	F	F
0.7239229024943299	0.3333333333333357	0.1468479604449939	F	F	F
0.7239229024943299	0.3333333333333357	0.2932018493337858	T	T	T
0.8905895691609942	0.5000000000000000	0.0734239802224934	F	F	F
0.8905895691609942	0.5000000000000000	0.2208972872956667	T	T	T
0.0572562358276656	0.6666666666666643	0.0000000000000000	F	F	F
0.0572562358276656	0.6666666666666643	0.1468479604449939	F	F	F
0.0572562358276656	0.6666666666666643	0.2932018493337858	T	T	T
0.2239229024943299	0.8333333333333357	0.0734239802224934	F	F	F
0.2239229024943299	0.8333333333333357	0.2208972872956667	T	T	T
0.3905895691609942	0.6666666666666643	0.0000000000000000	F	F	F

0.3905895691609942	0.6666666666666643	0.1468479604449939	F	F	F
0.3905895691609942	0.6666666666666643	0.2932018493337858	T	T	T
0.5572562358276656	0.8333333333333357	0.0734239802224934	F	F	F
0.5572562358276656	0.8333333333333357	0.2208972872956667	T	T	T
0.7239229024943299	0.6666666666666643	0.0000000000000000	F	F	F
0.7239229024943299	0.6666666666666643	0.1468479604449939	F	F	F
0.7239229024943299	0.6666666666666643	0.2932018493337858	T	T	T
0.8905895691609942	0.8333333333333357	0.0734239802224934	F	F	F
0.8905895691609942	0.8333333333333357	0.2208972872956667	T	T	T

Ag(511) within a 1 x 3 geometry POSCAR

Ag5111x3

1.0000000000000000

7.777999999999996	0.0000000000000000	0.0000000000000000
-1.6663200000000000	8.6613000000000007	0.0000000000000000
0.0000000000000000	0.0000000000000000	31.2020000000000017

45

Selective dynamics

Direct

0.0052360951708295	0.1585327837622543	0.9821806294468303	F	F	F
0.1534966737730201	0.1832403911652989	0.1104095891288992	F	F	F
0.2974912631361140	0.2089100691987592	0.2418177343428666	T	T	T
0.5655864401405871	0.0869502224405846	0.2870295762602008	T	T	T
0.3756056714237843	0.2201863461605100	0.9565412473559363	F	F	F
0.6348417841757694	0.0967637652546358	0.0078520607653374	F	F	F
0.5238662500259750	0.2448939535635546	0.0847702070380123	F	F	F
0.7831023627779601	0.1214713726576875	0.1360489712197932	F	F	F
0.9321092295256037	0.1476610734881054	0.2638553356559741	T	T	T
0.2645015695187851	0.0349832011360860	0.0334914428562243	F	F	F
0.4129492806718802	0.0609406887773578	0.1623863162051813	T	T	T
0.6735086657669038	0.2713122151485408	0.2128525718150336	T	T	T
0.745999824188444	0.2819553646681214	0.9309018652650494	F	F	F
0.8941319932658303	0.3066629720711660	0.0591308249471183	F	F	F
0.0459651572932876	0.3331651886344525	0.1882119200315043	T	T	T
0.0052360951708295	0.4918661170955829	0.9821806294468303	F	F	F
0.1534966737730201	0.5165737244986346	0.1104095891288992	F	F	F
0.2982720173558955	0.5417081082966581	0.2415510046465050	T	T	T
0.5671851023670456	0.4207120264804007	0.2870197001657365	T	T	T
0.3756056714237843	0.5535196794938386	0.9565412473559363	F	F	F
0.6348417841757694	0.4300970985879715	0.0078520607653374	F	F	F
0.5238662500259750	0.5782272868968832	0.0847702070380123	F	F	F
0.7831023627779601	0.4548047059910161	0.1360489712197932	F	F	F
0.9334720227570148	0.4811491417272772	0.2638679117880142	T	T	T
0.2645015695187851	0.3683165344694217	0.0334914428562243	F	F	F

0.4128748521157342	0.3939985478589905	0.1623326689242565	T	T	T
0.6738440032624756	0.6044444096529937	0.2127812759748979	T	T	T
0.7459999824188444	0.6152886980014571	0.9309018652650494	F	F	F
0.8941319932658303	0.6399963054045017	0.0591308249471183	F	F	F
0.0461518557335960	0.6663697050373570	0.1881535471561607	T	T	T
0.0052360951708295	0.8251994504289186	0.9821806294468303	F	F	F
0.1534966737730201	0.8499070578319632	0.1104095891288992	F	F	F
0.2976040494977051	0.8751300662230566	0.2414844018708741	T	T	T
0.5657674024544960	0.7535184696863145	0.2870171466423865	T	T	T
0.3756056714237843	0.8868530128271743	0.9565412473559363	F	F	F
0.6348417841757694	0.7634304319213072	0.0078520607653374	F	F	F
0.5238662500259750	0.9115606202302189	0.0847702070380123	F	F	F
0.7831023627779601	0.7881380393243518	0.1360489712197932	F	F	F
0.9322020241416886	0.8142382595360910	0.2637284321922804	T	T	T
0.2645015695187851	0.7016498678027574	0.0334914428562243	F	F	F
0.4131165813413755	0.7273260022804688	0.1623358997709657	T	T	T
0.6732826543474217	0.9379073067813557	0.2128569561021502	T	T	T
0.7459999824188444	0.9486220313347857	0.9309018652650494	F	F	F
0.8941319932658303	0.9733296387378374	0.0591308249471183	F	F	F
0.0460120380350904	0.0000490982441259	0.1882213251149515	T	T	T