

Electronic Supplementary Information

Structure Transition of Au₁₈ from Pyramid to Hollow-Cage during Soft-landing onto TiO₂ (110) Surface

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Part I: Supplementary Figures

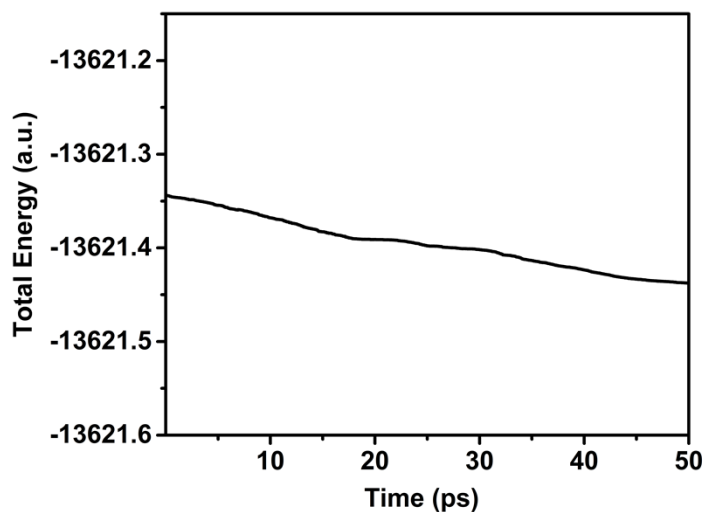


Figure S1 Time-evolution of the total energy of the Au₁₈/TiO₂ system during the soft-landing process of Au₁₈ onto TiO₂ (110) surface.

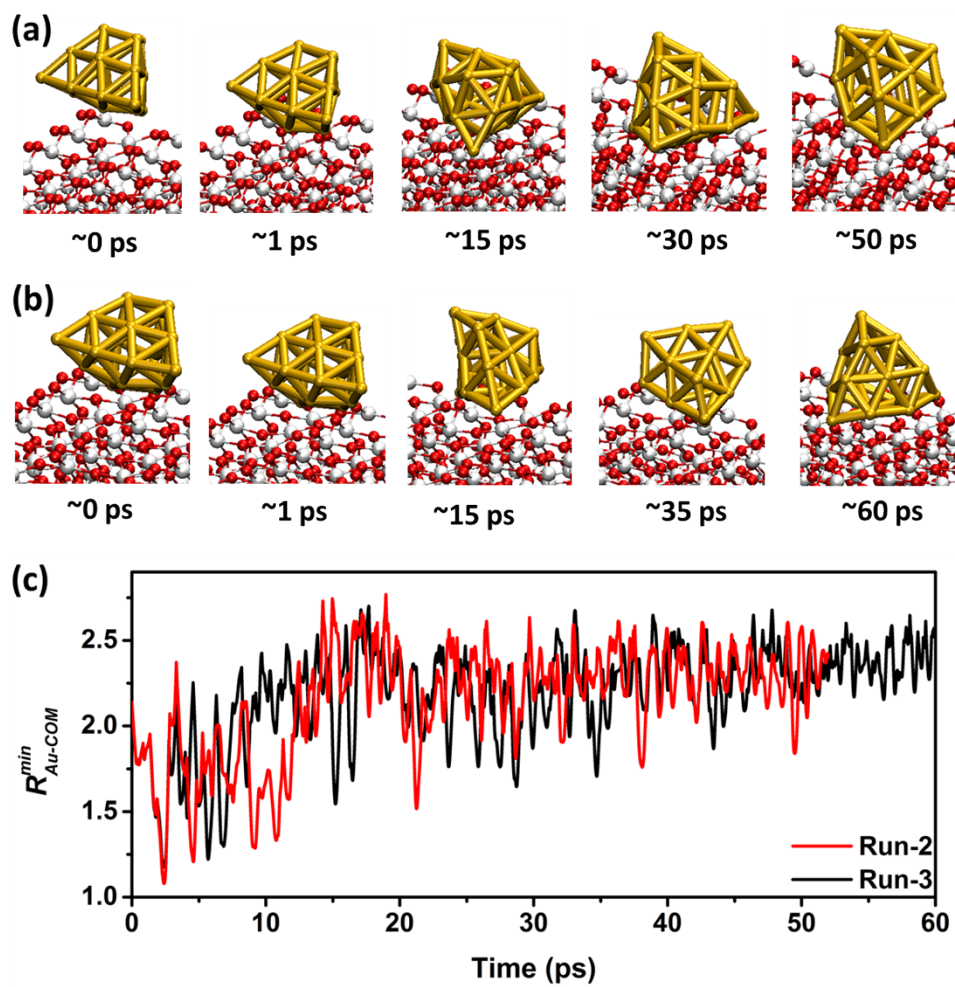


Figure S2 (a) and (b) present the snapshot structures from two independent BOMD simulations (Run-2 and Run-3, respectively) of the soft-landing of the Au₁₈ cluster onto the TiO₂ (110) surface. (c) Time-evolution of minimum distance of the Au atoms relative to the center of the mass (COM) of the Au₁₈ (R_{Au-COM}^{min}).

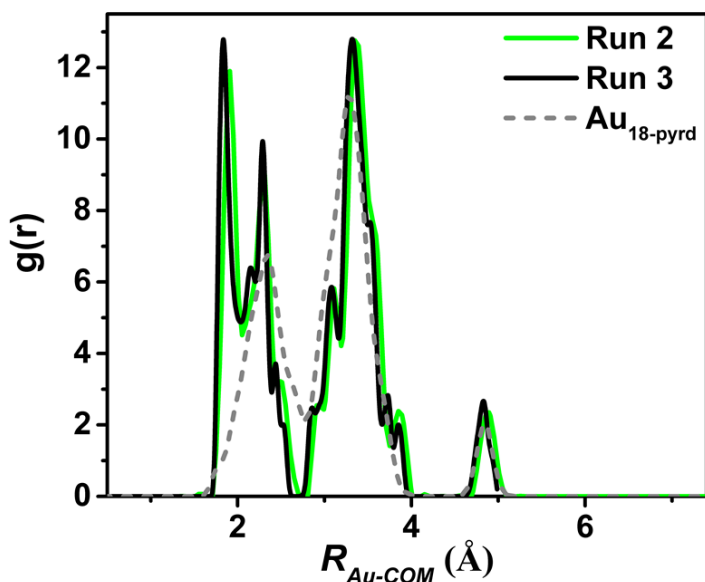


Figure S3 Computed $g(r)$ functions of the Au-COM distance for the pre-collision period ($t < 1$ ps) from the second and the third BOMD simulation Run 2 (green line) and Run 3 (black line). The dashed gray line shows the $g(r)$ functions for the bare Au_{18} -pyrd cluster (without TiO_2 support).

Part II: The coordinates for the optimized structures of the $\text{Au}_{18}/\text{TiO}_2$ systems obtained by soft-landing the Au_{18} cluster onto TiO_2 (110) surface

- (1) The optimized structure obtained from the first BOMD simulation of the soft-landing of Au_{18} onto TiO_2 (110) surface

Ti	0.7127383090	2.6404330640	2.9652979240
Ti	0.7127383090	-0.6080154890	6.2137464770
Ti	0.7314376185	2.7632727741	9.6396952151
Ti	0.7444427069	-0.5401312162	12.6024203879
Ti	2.1922383090	-0.6080154890	2.9652979240
Ti	2.1922383090	2.6404330640	6.2137464770
Ti	2.2183559859	-0.5292373391	9.4159039534
Ti	2.2044516352	2.6775947426	12.9535010940
O	0.7127383090	-0.6080154890	1.6971019120
O	0.7127383090	2.6404330640	4.9455504650
O	0.7264711255	-0.5885322786	8.2496681461
O	0.7011494899	2.7288478465	11.5098088340
O	0.7127383090	-0.6080154890	4.2334939360
O	0.7127383090	2.6404330640	7.4819424890
O	0.7396226795	-0.6265304663	10.7975333027
O	0.7717055106	2.6370818790	14.0670146346
O	2.1922383090	3.9086290760	2.9652979240

O	2.1922383090	0.6601805230	6.2137464770
O	2.1922335434	3.9801879375	9.4774897003
O	2.2470852692	0.6672444329	12.8779164811
O	2.1922383090	1.3722370520	2.9652979240
O	2.1922383090	4.6206856050	6.2137464770
O	2.1849859853	1.3731062281	9.5650387378
O	2.2250228822	4.7036560904	12.9670894339
Ti	3.6717383090	2.6404330640	2.9652979240
Ti	3.6717383090	-0.6080154890	6.2137464770
Ti	3.6883468798	2.6799960202	9.6214587182
Ti	3.6978271010	-0.6194548755	12.6003754659
Ti	5.1512383090	-0.6080154890	2.9652979240
Ti	5.1512383090	2.6404330640	6.2137464770
Ti	5.1744754953	-0.6337660803	9.4190827072
Ti	5.1168256393	2.6875785561	12.9653045761
O	3.6717383090	-0.6080154890	1.6971019120
O	3.6717383090	2.6404330640	4.9455504650
O	3.6966661364	-0.5601788472	8.2447900500
O	3.7042845059	2.7400044430	11.4796171470
O	3.6717383090	-0.6080154890	4.2334939360
O	3.6717383090	2.6404330640	7.4819424890
O	3.6990205151	-0.6265273003	10.7974660682
O	3.6651672276	2.6385576983	14.0588817620
O	5.1512383090	3.9086290760	2.9652979240
O	5.1512383090	0.6601805230	6.2137464770
O	5.1388561254	3.9847662606	9.4750690462
O	5.1375980725	0.6793748438	12.8916355856
O	5.1512383090	1.3722370520	2.9652979240
O	5.1512383090	4.6206856050	6.2137464770
O	5.1405967007	1.3748906095	9.5622718769
O	5.1467128507	4.7512496679	12.9861493467
Ti	6.6307383090	2.6404330640	2.9652979240
Ti	6.6307383090	-0.6080154890	6.2137464770
Ti	6.6411336669	2.6066623382	9.6322855797
Ti	6.6486892490	-0.5273478864	12.6279101477
Ti	8.1102383090	-0.6080154890	2.9652979240
Ti	8.1102383090	2.6404330640	6.2137464770
Ti	8.1268767240	-0.6440563909	9.4420479026
Ti	8.0516014744	2.7609555606	12.9726902909
O	6.6307383090	-0.6080154890	1.6971019120
O	6.6307383090	2.6404330640	4.9455504650
O	6.6564086708	-0.5784326585	8.2526280196
O	6.6226749198	2.7254205379	11.5016687794
O	6.6307383090	-0.6080154890	4.2334939360
O	6.6307383090	2.6404330640	7.4819424890
O	6.6210944076	-0.5855710063	10.8281898992
O	6.6126040224	2.7270599598	14.0608421964
O	8.1102383090	3.9086290760	2.9652979240
O	8.1102383090	0.6601805230	6.2137464770
O	8.0953128748	3.9814914694	9.4781374396
O	8.0958985674	0.6875544899	12.9819341760
O	8.1102383090	1.3722370520	2.9652979240
O	8.1102383090	4.6206856050	6.2137464770
O	8.0947092629	1.3732827679	9.5641679571
O	8.0993989567	4.7584884181	12.9006869425
Ti	9.5897383090	2.6404330640	2.9652979240
Ti	9.5897383090	-0.6080154890	6.2137464770
Ti	9.6088195667	2.6403320425	9.6162758112
Ti	9.6078384773	-0.5048510657	12.6305972734
Ti	11.0692383090	-0.6080154890	2.9652979240
Ti	11.0692383090	2.6404330640	6.2137464770
Ti	11.0812997188	-0.6358427802	9.4333253203
Ti	11.0081612772	2.6831597370	12.9533790998
O	9.5897383090	-0.6080154890	1.6971019120

O	9.5897383090	2.6404330640	4.9455504650
O	9.5866529477	-0.5897837551	8.2662045288
O	9.6160978339	2.6638941423	11.4796916042
O	9.5897383090	-0.6080154890	4.2334939360
O	9.5897383090	2.6404330640	7.4819424890
O	9.5775369492	-0.5773031965	10.8318114091
O	9.5709534641	2.7278724234	14.0531604059
O	11.0692383090	3.9086290760	2.9652979240
O	11.0692383090	0.6601805230	6.2137464770
O	11.0479109680	3.9844955191	9.4726555699
O	11.1303128502	0.6803517168	12.9846104289
O	11.0692383090	1.3722370520	2.9652979240
O	11.0692383090	4.6206856050	6.2137464770
O	11.0537176317	1.3708691538	9.4785700241
O	11.0421976397	4.7589208537	12.9830577200
Ti	12.5487383090	2.6404330640	2.9652979240
Ti	12.5487383090	-0.6080154890	6.2137464770
Ti	12.5720990368	2.6195826636	9.6237853450
Ti	12.5671346782	-0.6109605493	12.6320045797
Ti	14.0282383090	-0.6080154890	2.9652979240
Ti	14.0282383090	2.6404330640	6.2137464770
Ti	14.0418611279	-0.6240205957	9.4430956365
Ti	14.0561261413	2.6716098391	12.9461138251
O	12.5487383090	-0.6080154890	1.6971019120
O	12.5487383090	2.6404330640	4.9455504650
O	12.5506675937	-0.5917751210	8.2653373550
O	12.5315454105	2.7244730146	11.4480532901
O	12.5487383090	-0.6080154890	4.2334939360
O	12.5487383090	2.6404330640	7.4819424890
O	12.5338691328	-0.5824933514	10.8317813058
O	12.5362087554	2.7404499057	14.0581950853
O	14.0282383090	3.9086290760	2.9652979240
O	14.0282383090	0.6601805230	6.2137464770
O	14.0770495205	3.9567329881	9.4939198440
O	14.0130358934	0.6792262012	12.9811634210
O	14.0282383090	1.3722370520	2.9652979240
O	14.0282383090	4.6206856050	6.2137464770
O	14.0175869208	1.3675163697	9.5633919175
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Ti	15.5077383090	2.6404330640	2.9652979240
Ti	15.5077383090	-0.6080154890	6.2137464770
Ti	15.5339697511	2.6731008597	9.6402326999
Ti	15.5260792395	-0.5247168046	12.6346423220
Ti	16.9872383090	-0.6080154890	2.9652979240
Ti	16.9872383090	2.6404330640	6.2137464770
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Ti	17.0198999986	2.6958835873	13.0126449860
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O	15.5077383090	-0.6080154890	4.2334939360
O	15.5077383090	2.6404330640	7.4819424890
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O	15.4915105755	2.7219600809	14.0613558913
O	16.9872383090	3.9086290760	2.9652979240
O	16.9872383090	0.6601805230	6.2137464770
O	16.9801256930	3.9727976068	9.4789939641
O	17.0479704725	0.6767919143	12.9814776235
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O	16.9872383090	4.6206856050	6.2137464770
O	17.0440846661	1.3665567972	9.5585300246
O	17.0445986563	4.6951137506	12.9811310775
Ti	0.7127383090	9.1373301700	2.9652979240

Ti	0.7127383090	5.8888816170	6.2137464770
Ti	0.7350269301	9.2136114091	9.6454024451
Ti	0.7317487136	5.8975656724	12.6163217617
Ti	2.1922383090	5.8888816170	2.9652979240
Ti	2.1922383090	9.1373301700	6.2137464770
Ti	2.2081705372	5.9862745041	9.4252950356
Ti	2.1746916978	9.1320936515	12.9863066265
O	0.7127383090	5.8888816170	1.6971019120
O	0.7127383090	9.1373301700	4.9455504650
O	0.7325031925	5.9390066786	8.2459337052
O	0.7024202535	9.1724007961	11.5130795978
O	0.7127383090	5.8888816170	4.2334939360
O	0.7127383090	9.1373301700	7.4819424890
O	0.7428302584	5.9146299556	10.8038159642
O	0.6931821790	9.1622792284	14.0658226219
O	2.1922383090	10.4055261820	2.9652979240
O	2.1922383090	7.1570776290	6.2137464770
O	2.1854713878	10.5085757858	9.5565378906
O	2.1865649113	7.1372491590	12.9822372017
O	2.1922383090	7.8691341580	2.9652979240
O	2.1922383090	11.1175827100	6.2137464770
O	2.1863820126	7.8986721134	9.5609240276
O	2.1753421364	11.2084203650	12.9843532079
Ti	3.6717383090	9.1373301700	2.9652979240
Ti	3.6717383090	5.8888816170	6.2137464770
Ti	3.6986372689	9.2015583564	9.6464731301
Ti	3.6842435454	5.9277273531	12.6314398491
Ti	5.1512383090	5.8888816170	2.9652979240
Ti	5.1512383090	9.1373301700	6.2137464770
Ti	5.1611992796	5.8906184476	9.4312450344
Ti	5.1101545880	9.1999128888	12.9870068096
O	3.6717383090	5.8888816170	1.6971019120
O	3.6717383090	9.1373301700	4.9455504650
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O	5.1512383090	7.8691341580	2.9652979240
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O	5.1295444592	7.8932992222	9.5666322800
O	5.1316914811	11.2147094103	12.9846366650
Ti	6.6307383090	9.1373301700	2.9652979240
Ti	6.6307383090	5.8888816170	6.2137464770
Ti	6.6333166125	9.1160995548	9.6459555962
Ti	6.6274875887	5.9873147671	12.6267170534
Ti	8.1102383090	5.8888816170	2.9652979240
Ti	8.1102383090	9.1373301700	6.2137464770
Ti	8.1242663959	5.8702718421	9.4255031762
Ti	8.0514635856	9.2151762977	12.9866443006
O	6.6307383090	5.8888816170	1.6971019120
O	6.6307383090	9.1373301700	4.9455504650
O	6.6293263900	5.9486483217	8.2577430915
O	6.6112853990	9.1636558825	11.5172482495
O	6.6307383090	5.8888816170	4.2334939360
O	6.6307383090	9.1373301700	7.4819424890
O	6.6131645531	5.9442570742	10.8283957440
O	6.6065374722	9.2530960981	14.0681519192
O	8.1102383090	10.4055261820	2.9652979240

O	8.1102383090	7.1570776290	6.2137464770
O	8.0947399170	10.4374513636	9.5610937235
O	8.0923730876	7.1973917843	12.9850171797
O	8.1102383090	7.8691341580	2.9652979240
O	8.1102383090	11.1175827100	6.2137464770
O	8.0944530076	7.8852237967	9.5621242286
O	8.1006417554	11.2164254755	12.9812114283
Ti	9.5897383090	9.1373301700	2.9652979240
Ti	9.5897383090	5.8888816170	6.2137464770
Ti	9.6011850339	9.1077469056	9.6475179164
Ti	9.6079637239	6.0054456210	12.6153692622
Ti	11.0692383090	5.8888816170	2.9652979240
Ti	11.0692383090	9.1373301700	6.2137464770
Ti	11.1020923729	5.8745248054	9.4175040702
Ti	11.0066480305	9.1951249501	12.9753476766
O	9.5897383090	5.8888816170	1.6971019120
O	9.5897383090	9.1373301700	4.9455504650
O	9.5899102785	5.9472171858	8.2556938863
O	9.5781454313	9.1657594220	11.5122589154
O	9.5897383090	5.8888816170	4.2334939360
O	9.5897383090	9.1373301700	7.4819424890
O	9.5764224839	5.9434015197	10.8252077556
O	9.5759628792	9.1627847210	14.0635801248
O	11.0692383090	10.4055261820	2.9652979240
O	11.0692383090	7.1570776290	6.2137464770
O	11.0531172137	10.4351802877	9.4766652096
O	11.1286021707	7.1972951906	12.8876256394
O	11.0692383090	7.8691341580	2.9652979240
O	11.0692383090	11.1175827100	6.2137464770
O	11.0697489434	7.8776140517	9.5642826289
O	11.0539276494	11.2114910300	12.9835167626
Ti	12.5487383090	9.1373301700	2.9652979240
Ti	12.5487383090	5.8888816170	6.2137464770
Ti	12.5844155610	9.1215762884	9.6248066258
Ti	12.5786910695	5.8889374023	12.6478075755
Ti	14.0282383090	5.8888816170	2.9652979240
Ti	14.0282383090	9.1373301700	6.2137464770
Ti	14.0646607960	5.8944863656	9.4866005699
Ti	14.0296120040	9.1976089405	12.9415636349
O	12.5487383090	5.8888816170	1.6971019120
O	12.5487383090	9.1373301700	4.9455504650
O	12.6006345977	5.9432386329	8.2785355411
O	12.6076364443	9.2563744944	11.4464091579
O	12.5487383090	5.8888816170	4.2334939360
O	12.5487383090	9.1373301700	7.4819424890
O	12.5345792910	5.8526384058	10.8293449369
O	12.5443414910	9.1582102246	14.0546552671
O	14.0282383090	10.4055261820	2.9652979240
O	14.0282383090	7.1570776290	6.2137464770
O	14.0832799927	10.4546011420	9.4696390340
O	14.0399624765	7.1630097124	12.8666443525
O	14.0282383090	7.8691341580	2.9652979240
O	14.0282383090	11.1175827100	6.2137464770
O	14.0830999673	7.8804775013	9.5650787812
O	14.0929410038	11.2051824296	12.8963945416
Ti	15.5077383090	9.1373301700	2.9652979240
Ti	15.5077383090	5.8888816170	6.2137464770
Ti	15.5304814660	9.1963479780	9.6281871592
Ti	15.5426096291	5.9780903125	12.6648740800
Ti	16.9872383090	5.8888816170	2.9652979240
Ti	16.9872383090	9.1373301700	6.2137464770
Ti	17.0054080691	5.9890474742	9.4265024036
Ti	16.9903251664	9.2053857867	12.9559838704
O	15.5077383090	5.8888816170	1.6971019120

O	15.5077383090	9.1373301700	4.9455504650
O	15.5115869737	5.9428478296	8.2706117220
O	15.5461715864	9.1851407712	11.4835287884
O	15.5077383090	5.8888816170	4.2334939360
O	15.5077383090	9.1373301700	7.4819424890
O	15.5754862970	5.9395274569	10.8339022471
O	15.4913263327	9.1614355969	14.0555732636
O	16.9872383090	10.4055261820	2.9652979240
O	16.9872383090	7.1570776290	6.2137464770
O	17.0204048273	10.4847349870	9.4898489820
O	17.0328190454	7.1606969864	12.8977024378
O	16.9872383090	7.8691341580	2.9652979240
O	16.9872383090	11.1175827100	6.2137464770
O	17.0430371321	7.8911788624	9.5555979942
O	16.9723737256	11.2193463708	12.9819167915
Ti	0.7127383090	15.6342272750	2.9652979240
Ti	0.7127383090	12.3857787220	6.2137464770
Ti	0.7397417113	15.7440045193	9.6349490214
Ti	0.7184983286	12.4132615276	12.6328617198
Ti	2.1922383090	12.3857787220	2.9652979240
Ti	2.1922383090	15.6342272750	6.2137464770
Ti	2.2105499005	12.4467875514	9.4384552081
Ti	2.1999922482	15.6636185886	12.9851352645
O	0.7127383090	12.3857787220	1.6971019120
O	0.7127383090	15.6342272750	4.9455504650
O	0.7423479508	12.4459171144	8.2504666442
O	0.7002108971	15.7807923785	11.5075949226
O	0.7127383090	12.3857787220	4.2334939360
O	0.7127383090	15.6342272750	7.4819424890
O	0.7027725403	12.4654612722	10.8302927789
O	0.7018747895	15.6889202122	14.0617471065
O	2.1922383090	16.9024232870	2.9652979240
O	2.1922383090	13.6539747350	6.2137464770
O	2.2537626781	16.9579641068	9.4765690412
O	2.1805637545	13.6557041468	12.9839681278
O	2.1922383090	14.3660312630	2.9652979240
O	2.1922383090	17.6144798160	6.2137464770
O	2.1776202607	14.4103925863	9.5671128043
O	2.1778361371	17.7303457778	12.9855140774
Ti	3.6717383090	15.6342272750	2.9652979240
Ti	3.6717383090	12.3857787220	6.2137464770
Ti	3.6827222290	15.6512305925	9.6454388520
Ti	3.6648217113	12.4187289644	12.6352103261
Ti	5.1512383090	12.3857787220	2.9652979240
Ti	5.1512383090	15.6342272750	6.2137464770
Ti	5.1702003596	12.4203556701	9.4280929418
Ti	5.1755718488	15.6600885191	13.0168479061
O	3.6717383090	12.3857787220	1.6971019120
O	3.6717383090	15.6342272750	4.9455504650
O	3.6772381194	12.4527161019	8.2605082247
O	3.7324626392	15.6894237029	11.5152900701
O	3.6717383090	12.3857787220	4.2334939360
O	3.6717383090	15.6342272750	7.4819424890
O	3.6598249670	12.4677839481	10.8338904608
O	3.6615433223	15.7729254740	14.0644684732
O	5.1512383090	16.9024232870	2.9652979240
O	5.1512383090	13.6539747350	6.2137464770
O	5.1499478495	16.9528646938	9.4756287473
O	5.1347583963	13.6511870313	12.9887521651
O	5.1512383090	14.3660312630	2.9652979240
O	5.1512383090	17.6144798160	6.2137464770
O	5.1794512672	14.3634026948	9.5395187595
O	5.2156785083	17.7285844334	12.9889922482
Ti	6.6307383090	15.6342272750	2.9652979240

Ti	6.6307383090	12.3857787220	6.2137464770
Ti	6.6530271658	15.6346946227	9.6833345092
Ti	6.6362945168	12.4208272171	12.6393238287
Ti	8.1102383090	12.3857787220	2.9652979240
Ti	8.1102383090	15.6342272750	6.2137464770
Ti	8.1188022528	12.3305448471	9.4433006024
Ti	8.1531561490	15.7335155298	13.0052874796
O	6.6307383090	12.3857787220	1.6971019120
O	6.6307383090	15.6342272750	4.9455504650
O	6.6417337119	12.3939968654	8.2585483781
O	6.6150005234	15.6901020735	11.5229019222
O	6.6307383090	12.3857787220	4.2334939360
O	6.6307383090	15.6342272750	7.4819424890
O	6.6112763604	12.3787711552	10.8363031742
O	6.6833903321	15.6878023878	14.0738329198
O	8.1102383090	16.9024232870	2.9652979240
O	8.1102383090	13.6539747350	6.2137464770
O	8.1012037717	16.9502358216	9.5617607126
O	8.0956645550	13.6486313148	12.9834280619
O	8.1102383090	14.3660312630	2.9652979240
O	8.1102383090	17.6144798160	6.2137464770
O	8.0941825204	14.3381259983	9.5646202723
O	8.1731244897	17.7331705552	12.9829940687
Ti	9.5897383090	15.6342272750	2.9652979240
Ti	9.5897383090	12.3857787220	6.2137464770
Ti	9.6044254043	15.5658212811	9.6503068964
Ti	9.5978952078	12.4953851723	12.6296628218
Ti	11.0692383090	12.3857787220	2.9652979240
Ti	11.0692383090	15.6342272750	6.2137464770
Ti	11.0841092251	12.3270871948	9.4213422639
Ti	11.0994919255	15.6581085046	12.9535746826
O	9.5897383090	12.3857787220	1.6971019120
O	9.5897383090	15.6342272750	4.9455504650
O	9.5805270601	12.3828211695	8.2712558504
O	9.5716648515	15.5987444149	11.5108751356
O	9.5897383090	12.3857787220	4.2334939360
O	9.5897383090	15.6342272750	7.4819424890
O	9.5756434090	12.3780355655	10.8364777054
O	9.6501318282	15.6861043040	14.0625331998
O	11.0692383090	16.9024232870	2.9652979240
O	11.0692383090	13.6539747350	6.2137464770
O	11.0510050448	16.9473587914	9.5612232993
O	11.1342566331	13.6432972921	12.8920494770
O	11.0692383090	14.3660312630	2.9652979240
O	11.0692383090	17.6144798160	6.2137464770
O	11.0571792484	14.3334765963	9.5626246939
O	11.0565597161	17.7221141754	12.8982802280
Ti	12.5487383090	15.6342272750	2.9652979240
Ti	12.5487383090	12.3857787220	6.2137464770
Ti	12.5620453978	15.6339774355	9.6346266767
Ti	12.5728743882	12.3426330400	12.5848821107
Ti	14.0282383090	12.3857787220	2.9652979240
Ti	14.0282383090	15.6342272750	6.2137464770
Ti	14.0529065202	12.4124288248	9.3905623524
Ti	14.0469303127	15.6566133353	12.9877578906
O	12.5487383090	12.3857787220	1.6971019120
O	12.5487383090	15.6342272750	4.9455504650
O	12.5378101531	12.3813908330	8.2314865562
O	12.5801003811	15.6656694030	11.4796508021
O	12.5487383090	12.3857787220	4.2334939360
O	12.5487383090	15.6342272750	7.4819424890
O	12.5875936956	12.3703646162	10.7838964543
O	12.5406500221	15.6927372713	14.0562394040
O	14.0282383090	16.9024232870	2.9652979240

O	14.0282383090	13.6539747350	6.2137464770
O	14.0130203810	16.9526233514	9.5582434782
O	14.0121507902	13.6389582876	12.9805602128
O	14.0282383090	14.3660312630	2.9652979240
O	14.0282383090	17.6144798160	6.2137464770
O	14.0160327520	14.3442755347	9.4776725156
O	14.0813212423	17.7273166867	12.9823103965
Ti	15.5077383090	15.6342272750	2.9652979240
Ti	15.5077383090	12.3857787220	6.2137464770
Ti	15.5443099829	15.6515009619	9.6373120688
Ti	15.5342071550	12.5072162254	12.5919133665
Ti	16.9872383090	12.3857787220	2.9652979240
Ti	16.9872383090	15.6342272750	6.2137464770
Ti	17.0188606598	12.4452413845	9.4230466660
Ti	17.0020414914	15.7357447401	12.9771770812
O	15.5077383090	12.3857787220	1.6971019120
O	15.5077383090	15.6342272750	4.9455504650
O	15.5433676363	12.4371242052	8.2418823928
O	15.4919424600	15.6816925050	11.4997352608
O	15.5077383090	12.3857787220	4.2334939360
O	15.5077383090	15.6342272750	7.4819424890
O	15.5284263428	12.4476611630	10.7887856937
O	15.4986097082	15.6868671238	14.0623691053
O	16.9872383090	16.9024232870	2.9652979240
O	16.9872383090	13.6539747350	6.2137464770
O	16.9656329997	16.9567077551	9.4750934937
O	17.0101565289	13.6804670724	12.9243254659
O	16.9872383090	14.3660312630	2.9652979240
O	16.9872383090	17.6144798160	6.2137464770
O	17.0191748050	14.3899992811	9.5451802032
O	16.9726797662	17.7369265878	12.9840616650
Au	14.8087504795	4.6559008357	19.9826611806
Au	14.2046392130	8.9342947222	21.1643041675
Au	17.6399016780	6.9807563968	16.2974509983
Au	12.7969286897	7.3777700880	15.9385345363
Au	14.6515748113	3.4323840376	17.5112524255
Au	12.7919202074	6.5370472457	20.6907134410
Au	17.7471446817	9.2659421152	17.9501963139
Au	16.9699913340	4.8583945316	18.0392507059
Au	15.2787709624	8.5958357158	16.6417161937
Au	16.8126458536	8.1525154930	20.3768571660
Au	15.2067850975	5.8037075792	15.9563623927
Au	13.1789522047	8.3938559265	18.5524765116
Au	17.4381762177	5.3578975687	20.7725171257
Au	12.7432040686	4.4660117684	15.6437524685
Au	12.8536068352	5.6098508989	18.1222329454
Au	15.3334263219	10.1640898953	18.9649488174
Au	18.8143632786	6.8348888035	18.8653466859
Au	15.2675956924	6.4943279773	22.0605826634

(2) The optimized structure obtained from the second BOMD simulation of the soft-landing of Au₁₈ onto TiO₂(110) surface

Ti	0.7127383090	2.6404330640	2.9652979240
Ti	0.7127383090	-0.6080154890	6.2137464770
Ti	0.7249055339	2.5664054620	9.6893302997
Ti	0.7236199112	-0.6636204219	12.6316547294

Ti	2.1922383090	-0.6080154890	2.9652979240
Ti	2.1922383090	2.6404330640	6.2137464770
Ti	2.2042432029	-0.7306743414	9.4283459451
Ti	2.2199717168	2.5849671926	13.0232067903
O	0.7127383090	-0.6080154890	1.6971019120
O	0.7127383090	2.6404330640	4.9455504650
O	0.7170966974	-0.6669599251	8.2636132224
O	0.6969169901	2.6256962286	11.5281351707
O	0.7127383090	-0.6080154890	4.2334939360
O	0.7127383090	2.6404330640	7.4819424890
O	0.6973667636	-0.6787778341	10.8370252176
O	0.7395787428	2.5662243721	14.1044919053
O	2.1922383090	3.9086290760	2.9652979240
O	2.1922383090	0.6601805230	6.2137464770
O	2.1783652610	3.8903397856	9.5662023765
O	2.1769060776	0.5743241108	12.9791591729
O	2.1922383090	1.3722370520	2.9652979240
O	2.1922383090	4.6206856050	6.2137464770
O	2.1758646009	1.2831279299	9.5620546894
O	2.1781243981	4.5852451348	12.9859818988
Ti	3.6717383090	2.6404330640	2.9652979240
Ti	3.6717383090	-0.6080154890	6.2137464770
Ti	3.6889837178	2.5037637060	9.6303167801
Ti	3.6998985133	-0.6173894385	12.5833977622
Ti	5.1512383090	-0.6080154890	2.9652979240
Ti	5.1512383090	2.6404330640	6.2137464770
Ti	5.1665932753	-0.7310576141	9.3856464565
Ti	5.1777413558	2.5796260862	12.9541457812
O	3.6717383090	-0.6080154890	1.6971019120
O	3.6717383090	2.6404330640	4.9455504650
O	3.6545936726	-0.6791946995	8.2281645392
O	3.7320019104	2.5394915766	11.5094982538
O	3.6717383090	-0.6080154890	4.2334939360
O	3.6717383090	2.6404330640	7.4819424890
O	3.6974491414	-0.6134740804	10.7868989106
O	3.7291524386	2.5409619916	14.0690494184
O	5.1512383090	3.9086290760	2.9652979240
O	5.1512383090	0.6601805230	6.2137464770
O	5.1367730469	3.8894522316	9.4790483184
O	5.2131623861	0.5562388175	12.9745127321
O	5.1512383090	1.3722370520	2.9652979240
O	5.1512383090	4.6206856050	6.2137464770
O	5.1377880808	1.2845663588	9.4676084054
O	5.1437851581	4.5846491835	12.9777749003
Ti	6.6307383090	2.6404330640	2.9652979240
Ti	6.6307383090	-0.6080154890	6.2137464770
Ti	6.6563272917	2.5665538489	9.6007260716
Ti	6.6464675748	-0.6823487493	12.5598294440
Ti	8.1102383090	-0.6080154890	2.9652979240
Ti	8.1102383090	2.6404330640	6.2137464770
Ti	8.1323763899	-0.6318417479	9.4147834752
Ti	8.1316662210	2.5040974864	12.9094575965
O	6.6307383090	-0.6080154890	1.6971019120
O	6.6307383090	2.6404330640	4.9455504650
O	6.6487194963	-0.6719887549	8.2339223399
O	6.6198913797	2.5356498962	11.4472938804
O	6.6307383090	-0.6080154890	4.2334939360
O	6.6307383090	2.6404330640	7.4819424890
O	6.6183627435	-0.5922054558	10.7572688433
O	6.6974546195	2.5381485614	14.0529704982
O	8.1102383090	3.9086290760	2.9652979240
O	8.1102383090	0.6601805230	6.2137464770
O	8.0973256503	3.8926707261	9.5666969727
O	8.1637865988	0.5058896648	12.8896443597

O	8.1102383090	1.3722370520	2.9652979240
O	8.1102383090	4.6206856050	6.2137464770
O	8.1567832711	1.2958588113	9.4750494254
O	8.0952438490	4.5747244589	12.8857922223
Ti	9.5897383090	2.6404330640	2.9652979240
Ti	9.5897383090	-0.6080154890	6.2137464770
Ti	9.6192839349	2.6679415653	9.6172191856
Ti	9.6202878440	-0.7472523063	12.5569205669
Ti	11.0692383090	-0.6080154890	2.9652979240
Ti	11.0692383090	2.6404330640	6.2137464770
Ti	11.0980895285	-0.6241414127	9.3580307110
Ti	11.1145047766	2.5569777017	12.9408694117
O	9.5897383090	-0.6080154890	1.6971019120
O	9.5897383090	2.6404330640	4.9455504650
O	9.5776147170	-0.6801997489	8.2156697299
O	9.6214508628	2.5701475641	11.4760440904
O	9.5897383090	-0.6080154890	4.2334939360
O	9.5897383090	2.6404330640	7.4819424890
O	9.6520005542	-0.6802893971	10.7537593536
O	9.5774491510	2.5337109783	14.0599873053
O	11.0692383090	3.9086290760	2.9652979240
O	11.0692383090	0.6601805230	6.2137464770
O	11.1250767678	3.8900744514	9.5585076983
O	11.0513392236	0.5066705044	12.9783549184
O	11.0692383090	1.3722370520	2.9652979240
O	11.0692383090	4.6206856050	6.2137464770
O	11.0639365383	1.2887129502	9.4679695578
O	11.1219152850	4.5756598623	12.9818801984
Ti	12.5487383090	2.6404330640	2.9652979240
Ti	12.5487383090	-0.6080154890	6.2137464770
Ti	12.5636606779	2.5864201813	9.6286135457
Ti	12.5590147180	-0.6354627871	12.5875477268
Ti	14.0282383090	-0.6080154890	2.9652979240
Ti	14.0282383090	2.6404330640	6.2137464770
Ti	14.0578666052	-0.6467388405	9.4269025341
Ti	14.0532599160	2.5797409755	13.0196426115
O	12.5487383090	-0.6080154890	1.6971019120
O	12.5487383090	2.6404330640	4.9455504650
O	12.6063828625	-0.6734804732	8.2216978703
O	12.5323154035	2.5330965105	11.5127989063
O	12.5487383090	-0.6080154890	4.2334939360
O	12.5487383090	2.6404330640	7.4819424890
O	12.5658746242	-0.6143396787	10.7832365847
O	12.5308456807	2.5357114098	14.0673081117
O	14.0282383090	3.9086290760	2.9652979240
O	14.0282383090	0.6601805230	6.2137464770
O	14.0130178547	3.8899423202	9.5660298967
O	14.0181729963	0.5727263161	12.9826468355
O	14.0282383090	1.3722370520	2.9652979240
O	14.0282383090	4.6206856050	6.2137464770
O	14.0472238685	1.3032254886	9.4853159756
O	14.0133722445	4.5833517787	12.9845004976
Ti	15.5077383090	2.6404330640	2.9652979240
Ti	15.5077383090	-0.6080154890	6.2137464770
Ti	15.5333484516	2.5608682171	9.6831229989
Ti	15.5154351668	-0.6476190953	12.6359589877
Ti	16.9872383090	-0.6080154890	2.9652979240
Ti	16.9872383090	2.6404330640	6.2137464770
Ti	17.0009617843	-0.7180196491	9.4360878166
Ti	17.0107761641	2.5807241847	13.0326483020
O	15.5077383090	-0.6080154890	1.6971019120
O	15.5077383090	2.6404330640	4.9455504650
O	15.5363344543	-0.6551214585	8.2527048906
O	15.4871128669	2.5385813226	11.5263010076

O	15.5077383090	-0.6080154890	4.2334939360
O	15.5077383090	2.6404330640	7.4819424890
O	15.4939108447	-0.6768386414	10.8349674904
O	15.5181864754	2.5945687306	14.1055132274
O	16.9872383090	3.9086290760	2.9652979240
O	16.9872383090	0.6601805230	6.2137464770
O	16.9727519515	3.8902290998	9.5641632209
O	16.9781691088	0.5755001120	12.9802645967
O	16.9872383090	1.3722370520	2.9652979240
O	16.9872383090	4.6206856050	6.2137464770
O	16.9800524949	1.2864038843	9.5628575965
O	16.9701652025	4.5846565049	12.9854561575
Ti	0.7127383090	9.1373301700	2.9652979240
Ti	0.7127383090	5.8888816170	6.2137464770
Ti	0.7228601481	9.1013022154	9.6293874048
Ti	0.7159859923	5.8178885519	12.6316947672
Ti	2.1922383090	5.8888816170	2.9652979240
Ti	2.1922383090	9.1373301700	6.2137464770
Ti	2.2086029869	5.7832022822	9.4478484541
Ti	2.1193491788	9.0951699857	12.9567769248
O	0.7127383090	5.8888816170	1.6971019120
O	0.7127383090	9.1373301700	4.9455504650
O	0.7028114646	5.8492933153	8.2775573674
O	0.6935574577	9.1538295032	11.5097079941
O	0.7127383090	5.8888816170	4.2334939360
O	0.7127383090	9.1373301700	7.4819424890
O	0.6931074847	5.8456022361	10.8357598950
O	0.6944136425	9.0618169821	14.0577695485
O	2.1922383090	10.4055261820	2.9652979240
O	2.1922383090	7.1570776290	6.2137464770
O	2.1782158717	10.4169402057	9.5640463615
O	2.1757373722	7.0389538753	12.8981061984
O	2.1922383090	7.8691341580	2.9652979240
O	2.1922383090	11.1175827100	6.2137464770
O	2.1733013296	7.8089606194	9.5625835267
O	2.1782780379	11.1110600709	12.9839436435
Ti	3.6717383090	9.1373301700	2.9652979240
Ti	3.6717383090	5.8888816170	6.2137464770
Ti	3.6787805146	9.0307228880	9.6298008651
Ti	3.6864639299	5.8207207846	12.6331952878
Ti	5.1512383090	5.8888816170	2.9652979240
Ti	5.1512383090	9.1373301700	6.2137464770
Ti	5.1799803053	5.7743308094	9.4235622855
Ti	5.1577961851	9.1022008370	12.9268315618
O	3.6717383090	5.8888816170	1.6971019120
O	3.6717383090	9.1373301700	4.9455504650
O	3.6584621178	5.8504092989	8.2756435561
O	3.7049257271	9.1114272696	11.4761126441
O	3.6717383090	5.8888816170	4.2334939360
O	3.6717383090	9.1373301700	7.4819424890
O	3.6615904014	5.8426793984	10.8290208661
O	3.6502691782	9.0595124855	14.0621226196
O	5.1512383090	10.4055261820	2.9652979240
O	5.1512383090	7.1570776290	6.2137464770
O	5.1922455186	10.3927004693	9.4897516971
O	5.1314135015	7.0419981076	12.8927060245
O	5.1512383090	7.8691341580	2.9652979240
O	5.1512383090	11.1175827100	6.2137464770
O	5.1402521152	7.8018897474	9.4763194011
O	5.1370570874	11.1048358277	12.9828005622
Ti	6.6307383090	9.1373301700	2.9652979240
Ti	6.6307383090	5.8888816170	6.2137464770
Ti	6.6540612771	9.0366381868	9.6303855688
Ti	6.6530218725	5.8289460199	12.6647299223

Ti	8.1102383090	5.8888816170	2.9652979240
Ti	8.1102383090	9.1373301700	6.2137464770
Ti	8.1352676554	5.8783976475	9.4982222756
Ti	8.1249818945	9.0900429897	13.0170026059
O	6.6307383090	5.8888816170	1.6971019120
O	6.6307383090	9.1373301700	4.9455504650
O	6.6842019146	5.8519942663	8.2815148152
O	6.6147763108	9.0667705537	11.5053524442
O	6.6307383090	5.8888816170	4.2334939360
O	6.6307383090	9.1373301700	7.4819424890
O	6.6088543649	5.8473631756	10.8365455290
O	6.6113655513	9.0626146152	14.0600547966
O	8.1102383090	10.4055261820	2.9652979240
O	8.1102383090	7.1570776290	6.2137464770
O	8.1010095769	10.4108042887	9.5705344873
O	8.1508381416	7.0519206533	12.8863979321
O	8.1102383090	7.8691341580	2.9652979240
O	8.1102383090	11.1175827100	6.2137464770
O	8.1645263989	7.8086363535	9.5644317069
O	8.0930903075	11.1067498541	12.9833596984
Ti	9.5897383090	9.1373301700	2.9652979240
Ti	9.5897383090	5.8888816170	6.2137464770
Ti	9.6232794852	9.1810593147	9.6979941597
Ti	9.5989072441	5.7858930617	12.6602360000
Ti	11.0692383090	5.8888816170	2.9652979240
Ti	11.0692383090	9.1373301700	6.2137464770
Ti	11.0826943938	5.9037907236	9.4270167216
Ti	11.0467646175	9.0379861659	13.0468919444
O	9.5897383090	5.8888816170	1.6971019120
O	9.5897383090	9.1373301700	4.9455504650
O	9.5816076707	5.8455513901	8.2831146014
O	9.6132357498	9.0960309668	11.5611815177
O	9.5897383090	5.8888816170	4.2334939360
O	9.5897383090	9.1373301700	7.4819424890
O	9.6549185061	5.8410586342	10.8396239023
O	9.5699802472	9.0643106640	14.1458275640
O	11.0692383090	10.4055261820	2.9652979240
O	11.0692383090	7.1570776290	6.2137464770
O	11.0635864975	10.4127102043	9.5651049890
O	11.0585699979	7.0277886773	12.9894401776
O	11.0692383090	7.8691341580	2.9652979240
O	11.0692383090	11.1175827100	6.2137464770
O	11.0598052840	7.8110786693	9.5589734701
O	11.0533706519	11.1011933937	12.9854163028
Ti	12.5487383090	9.1373301700	2.9652979240
Ti	12.5487383090	5.8888816170	6.2137464770
Ti	12.5657248096	9.1140828734	9.6796054256
Ti	12.5546833477	5.8114254162	12.6317628727
Ti	14.0282383090	5.8888816170	2.9652979240
Ti	14.0282383090	9.1373301700	6.2137464770
Ti	14.0340708628	5.7998195753	9.4457987631
Ti	13.9773346230	9.0456845177	13.0190748698
O	12.5487383090	5.8888816170	1.6971019120
O	12.5487383090	9.1373301700	4.9455504650
O	12.5676891253	5.8584397719	8.2564404401
O	12.5311770029	9.0650775174	11.5345798563
O	12.5487383090	5.8888816170	4.2334939360
O	12.5487383090	9.1373301700	7.4819424890
O	12.5370822461	5.8479702285	10.8331350766
O	12.5305117136	9.0627172269	14.1402847614
O	14.0282383090	10.4055261820	2.9652979240
O	14.0282383090	7.1570776290	6.2137464770
O	14.0111471732	10.4098569977	9.5655683508
O	14.0153983617	7.0272564492	12.9876414751

O	14.0282383090	7.8691341580	2.9652979240
O	14.0282383090	11.1175827100	6.2137464770
O	14.0148815558	7.8039231420	9.5629910846
O	14.0063227442	11.1039654252	12.9849870248
Ti	15.5077383090	9.1373301700	2.9652979240
Ti	15.5077383090	5.8888816170	6.2137464770
Ti	15.5132306587	9.0408982070	9.6390408533
Ti	15.5154778199	5.8060825385	12.6376057479
Ti	16.9872383090	5.8888816170	2.9652979240
Ti	16.9872383090	9.1373301700	6.2137464770
Ti	16.9975986092	5.7987476078	9.4388294801
Ti	16.9268106073	9.0946332322	12.9666009388
O	15.5077383090	5.8888816170	1.6971019120
O	15.5077383090	9.1373301700	4.9455504650
O	15.4997429619	5.8511274822	8.2773504100
O	15.4914599684	9.0666192421	11.5172367462
O	15.5077383090	5.8888816170	4.2334939360
O	15.5077383090	9.1373301700	7.4819424890
O	15.4925988688	5.7643320976	10.8396835241
O	15.4851032936	9.0645268245	14.0671549575
O	16.9872383090	10.4055261820	2.9652979240
O	16.9872383090	7.1570776290	6.2137464770
O	16.9719656501	10.4095883288	9.4798596327
O	16.9704808236	7.0261162719	12.9829311345
O	16.9872383090	7.8691341580	2.9652979240
O	16.9872383090	11.1175827100	6.2137464770
O	16.9719998010	7.8026529811	9.5649492831
O	16.9661808570	11.1082437335	12.9867207219
Ti	0.7127383090	15.6342272750	2.9652979240
Ti	0.7127383090	12.3857787220	6.2137464770
Ti	0.7136951589	15.5560013043	9.6498310114
Ti	0.7060651151	12.3349470109	12.6297558254
Ti	2.1922383090	12.3857787220	2.9652979240
Ti	2.1922383090	15.6342272750	6.2137464770
Ti	2.2099825244	12.3241255785	9.4483239228
Ti	2.2206734758	15.6080747281	12.9488318573
O	0.7127383090	12.3857787220	1.6971019120
O	0.7127383090	15.6342272750	4.9455504650
O	0.7353009873	12.3650849828	8.2618607188
O	0.6874375932	15.5915869035	11.5138476916
O	0.7127383090	12.3857787220	4.2334939360
O	0.7127383090	15.6342272750	7.4819424890
O	0.6896930558	12.3725678187	10.8320607284
O	0.7644923090	15.5938832451	14.0610739276
O	2.1922383090	16.9024232870	2.9652979240
O	2.1922383090	13.6539747350	6.2137464770
O	2.1803011487	16.8735060264	9.5644661693
O	2.1755338505	13.5520218104	12.8968538247
O	2.1922383090	14.3660312630	2.9652979240
O	2.1922383090	17.6144798160	6.2137464770
O	2.1762593427	14.3098748936	9.5610929426
O	2.2523431595	17.6298207339	12.8926783656
Ti	3.6717383090	15.6342272750	2.9652979240
Ti	3.6717383090	12.3857787220	6.2137464770
Ti	3.6974540647	15.5319539028	9.6309641957
Ti	3.6723748181	12.3439526777	12.6342781198
Ti	5.1512383090	12.3857787220	2.9652979240
Ti	5.1512383090	15.6342272750	6.2137464770
Ti	5.1767656182	12.2652890662	9.4211702599
Ti	5.1605668737	15.5619504989	12.9843015306
O	3.6717383090	12.3857787220	1.6971019120
O	3.6717383090	15.6342272750	4.9455504650
O	3.6623986714	12.3704138020	8.2753061362
O	3.7023591016	15.5232251115	11.4876228893

O	3.6717383090	12.3857787220	4.2334939360
O	3.6717383090	15.6342272750	7.4819424890
O	3.7356674788	12.3716393725	10.8331622880
O	3.6580728424	15.5936980145	14.0577136320
O	5.1512383090	16.9024232870	2.9652979240
O	5.1512383090	13.6539747350	6.2137464770
O	5.1446164544	16.8759153451	9.5630327715
O	5.1357880418	13.5365566070	13.0750383682
O	5.1512383090	14.3660312630	2.9652979240
O	5.1512383090	17.6144798160	6.2137464770
O	5.1441098279	14.3136731712	9.4707063129
O	5.1437945894	17.6186581874	12.8863612898
Ti	6.6307383090	15.6342272750	2.9652979240
Ti	6.6307383090	12.3857787220	6.2137464770
Ti	6.6571340925	15.5353525785	9.6537873589
Ti	6.6312212443	12.3399695077	12.6404969806
Ti	8.1102383090	12.3857787220	2.9652979240
Ti	8.1102383090	15.6342272750	6.2137464770
Ti	8.1381766541	12.3513103322	9.4516102233
Ti	8.1203079878	15.5488237676	12.9954189254
O	6.6307383090	12.3857787220	1.6971019120
O	6.6307383090	15.6342272750	4.9455504650
O	6.6817888113	12.3756754056	8.2704335020
O	6.6101352473	15.4983522379	11.5107452503
O	6.6307383090	12.3857787220	4.2334939360
O	6.6307383090	15.6342272750	7.4819424890
O	6.6128992405	12.3762971655	10.8380550352
O	6.6193676046	15.5953883800	14.0649648568
O	8.1102383090	16.9024232870	2.9652979240
O	8.1102383090	13.6539747350	6.2137464770
O	8.0915978626	16.8735099356	9.5671257669
O	8.0958746961	13.5433795721	12.9853806907
O	8.1102383090	14.3660312630	2.9652979240
O	8.1102383090	17.6144798160	6.2137464770
O	8.1674848008	14.3142258540	9.5600865978
O	8.0951429532	17.5600419730	12.8822977394
Ti	9.5897383090	15.6342272750	2.9652979240
Ti	9.5897383090	12.3857787220	6.2137464770
Ti	9.6072061967	15.6538421012	9.6444182696
Ti	9.6098475036	12.3208846966	12.6431780805
Ti	11.0692383090	12.3857787220	2.9652979240
Ti	11.0692383090	15.6342272750	6.2137464770
Ti	11.0930405486	12.4323238088	9.4246066960
Ti	11.0823426524	15.5542294494	12.9831765546
O	9.5897383090	12.3857787220	1.6971019120
O	9.5897383090	15.6342272750	4.9455504650
O	9.5886276009	12.3645223563	8.2686870171
O	9.6471888805	15.5883767256	11.5056638762
O	9.5897383090	12.3857787220	4.2334939360
O	9.5897383090	15.6342272750	7.4819424890
O	9.6494565052	12.3743783650	10.8426045428
O	9.5742137457	15.5936878326	14.0645923103
O	11.0692383090	16.9024232870	2.9652979240
O	11.0692383090	13.6539747350	6.2137464770
O	11.1056456058	16.9040071248	9.4959547859
O	11.0537170294	13.5382176270	13.0718975771
O	11.0692383090	14.3660312630	2.9652979240
O	11.0692383090	17.6144798160	6.2137464770
O	11.0617284951	14.3238462201	9.4754011809
O	11.1042547299	17.5844512347	12.9130708492
Ti	12.5487383090	15.6342272750	2.9652979240
Ti	12.5487383090	12.3857787220	6.2137464770
Ti	12.5763905336	15.6341017402	9.6429936129
Ti	12.5516943273	12.3320842912	12.6447174632

Ti	14.0282383090	12.3857787220	2.9652979240
Ti	14.0282383090	15.6342272750	6.2137464770
Ti	14.0389460669	12.3313960873	9.4483207368
Ti	14.0296812532	15.6222901286	13.0006442421
O	12.5487383090	12.3857787220	1.6971019120
O	12.5487383090	15.6342272750	4.9455504650
O	12.5673678598	12.3588092975	8.2571299198
O	12.5329021765	15.5892618576	11.5124161079
O	12.5487383090	12.3857787220	4.2334939360
O	12.5487383090	15.6342272750	7.4819424890
O	12.5300500572	12.3765751338	10.8388706594
O	12.5411234562	15.5922267436	14.0696405815
O	14.0282383090	16.9024232870	2.9652979240
O	14.0282383090	13.6539747350	6.2137464770
O	14.0475136849	16.8939779492	9.5430249636
O	14.0115887440	13.5491399380	12.9841133548
O	14.0282383090	14.3660312630	2.9652979240
O	14.0282383090	17.6144798160	6.2137464770
O	14.0136944802	14.3158987836	9.5636463407
O	14.0138137072	17.6325968250	12.9831821287
Ti	15.5077383090	15.6342272750	2.9652979240
Ti	15.5077383090	12.3857787220	6.2137464770
Ti	15.5085753045	15.5565490498	9.6810396824
Ti	15.4866072272	12.3280046903	12.6384762101
Ti	16.9872383090	12.3857787220	2.9652979240
Ti	16.9872383090	15.6342272750	6.2137464770
Ti	17.0001943307	12.3172689028	9.4208570244
Ti	17.0111041108	15.5671302102	13.0182630912
O	15.5077383090	12.3857787220	1.6971019120
O	15.5077383090	15.6342272750	4.9455504650
O	15.4942944404	12.3757300381	8.2750439192
O	15.4933862527	15.5905122803	11.5232410510
O	15.5077383090	12.3857787220	4.2334939360
O	15.5077383090	15.6342272750	7.4819424890
O	15.4966660396	12.2909876656	10.8365383885
O	15.5000640194	15.5922293958	14.0698859753
O	16.9872383090	16.9024232870	2.9652979240
O	16.9872383090	13.6539747350	6.2137464770
O	16.9752884750	16.8723234369	9.5635731401
O	16.9696770971	13.5497100352	12.9866232237
O	16.9872383090	14.3660312630	2.9652979240
O	16.9872383090	17.6144798160	6.2137464770
O	16.9734502310	14.3116178827	9.4811839749
O	16.9751126406	17.6294922103	12.9876842081
Au	4.2659898159	5.0292540058	16.3929047622
Au	3.8428047948	7.8122540139	15.9990324957
Au	9.4219149629	7.0681548861	19.9915718712
Au	8.4418623751	8.1662069114	17.5230022880
Au	9.5801142846	3.0969104287	16.3007434788
Au	4.4628982227	6.8880974699	18.5221407243
Au	7.7934706513	4.6633124467	20.5238800185
Au	9.8935872940	4.6724882065	18.5395177379
Au	6.7609808277	8.1502083878	19.8417505568
Au	5.5531009358	4.2439164329	18.7921029448
Au	10.9968766636	7.0704684411	17.6943821567
Au	5.8797171029	9.1521933872	17.4442991565
Au	7.8966522900	2.7388766028	18.5493236732
Au	9.0749454316	5.8415529774	16.0006861492
Au	6.4951984922	6.7778293158	15.9036259202
Au	5.2871791500	5.9647475736	20.9839936723
Au	7.7156446838	6.9383232162	22.1457856738
Au	6.8417067145	3.9954330128	16.2275299636

- (3) The optimized structure obtained from the third BOMD simulation of the soft-landing of Au₁₈ onto TiO₂(110) surface

Ti	0.7127383090	2.6404330640	2.9652979240
Ti	0.7127383090	-0.6080154890	6.2137464770
Ti	0.7129639610	2.5796238023	9.6222180179
Ti	0.7099749189	-0.6465847010	12.5616025602
Ti	2.1922383090	-0.6080154890	2.9652979240
Ti	2.1922383090	2.6404330640	6.2137464770
Ti	2.2211363014	-0.6391818042	9.4225202650
Ti	2.1516614844	2.5917953151	12.9800046678
O	0.7127383090	-0.6080154890	1.6971019120
O	0.7127383090	2.6404330640	4.9455504650
O	0.7648906342	-0.5956691506	8.2205216760
O	0.6942441300	2.5396034971	11.5110789307
O	0.7127383090	-0.6080154890	4.2334939360
O	0.7127383090	2.6404330640	7.4819424890
O	0.6959349528	-0.5850045427	10.7565233877
O	0.6892198489	2.5387841984	14.0657321740
O	2.1922383090	3.9086290760	2.9652979240
O	2.1922383090	0.6601805230	6.2137464770
O	2.1704238099	3.9008372269	9.4782842625
O	2.1709492464	0.5701584134	12.9780849928
O	2.1922383090	1.3722370520	2.9652979240
O	2.1922383090	4.6206856050	6.2137464770
O	2.1877375198	1.3502440514	9.4790914899
O	2.1760141097	4.5979882595	12.9699663340
Ti	3.6717383090	2.6404330640	2.9652979240
Ti	3.6717383090	-0.6080154890	6.2137464770
Ti	3.6360503653	2.6702625328	9.6205852968
Ti	3.6542025906	-0.6397934999	12.6307425081
Ti	5.1512383090	-0.6080154890	2.9652979240
Ti	5.1512383090	2.6404330640	6.2137464770
Ti	5.1693406113	-0.5426242455	9.4333369401
Ti	5.0881753309	2.5999830909	12.9612810318
O	3.6717383090	-0.6080154890	1.6971019120
O	3.6717383090	2.6404330640	4.9455504650
O	3.6955236705	-0.6485571200	8.2514708227
O	3.6564498477	2.6305971509	11.5048278396
O	3.6717383090	-0.6080154890	4.2334939360
O	3.6717383090	2.6404330640	7.4819424890
O	3.6590352820	-0.5852402575	10.8299446602
O	3.6537198841	2.5413293689	14.0620445601
O	5.1512383090	3.9086290760	2.9652979240
O	5.1512383090	0.6601805230	6.2137464770
O	5.1350487200	3.9028788993	9.4764950870
O	5.1380417389	0.5823590666	12.9825524383
O	5.1512383090	1.3722370520	2.9652979240
O	5.1512383090	4.6206856050	6.2137464770
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Ti	6.6307383090	2.6404330640	2.9652979240
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Ti	6.6228546559	2.6711623994	9.6105426679
Ti	6.6214306182	-0.6262404073	12.6389954805
Ti	8.1102383090	-0.6080154890	2.9652979240
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Ti	8.1063955409	2.5652496379	12.8752968742
O	6.6307383090	-0.6080154890	1.6971019120
O	6.6307383090	2.6404330640	4.9455504650
O	6.6234319416	-0.6686637160	8.2604219088
O	6.6052547236	2.5370857859	11.4439769662
O	6.6307383090	-0.6080154890	4.2334939360
O	6.6307383090	2.6404330640	7.4819424890
O	6.6164983707	-0.6776503587	10.8343641295
O	6.6159346872	2.6343446916	14.0514494450
O	8.1102383090	3.9086290760	2.9652979240
O	8.1102383090	0.6601805230	6.2137464770
O	8.0947932019	3.8956571230	9.5634746155
O	8.0945965790	0.5680799243	12.9715922927
O	8.1102383090	1.3722370520	2.9652979240
O	8.1102383090	4.6206856050	6.2137464770
O	8.0912906322	1.2826952816	9.4711081146
O	8.0878713754	4.5763328513	12.7940916225
Ti	9.5897383090	2.6404330640	2.9652979240
Ti	9.5897383090	-0.6080154890	6.2137464770
Ti	9.6119009831	2.6634147953	9.6030868937
Ti	9.5967645483	-0.7179024360	12.6290279807
Ti	11.0692383090	-0.6080154890	2.9652979240
Ti	11.0692383090	2.6404330640	6.2137464770
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O	9.5768161681	-0.6751417813	8.2311006366
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O	9.5897383090	2.6404330640	7.4819424890
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O	9.5730461592	2.5432263283	13.9715874658
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O	11.0692383090	0.6601805230	6.2137464770
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O	11.0530847317	0.5014848509	12.9797759748
O	11.0692383090	1.3722370520	2.9652979240
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Ti	12.5487383090	2.6404330640	2.9652979240
Ti	12.5487383090	-0.6080154890	6.2137464770
Ti	12.5652404186	2.5773628771	9.6181506038
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Ti	14.0282383090	-0.6080154890	2.9652979240
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O	12.5487383090	2.6404330640	4.9455504650
O	12.5495412322	-0.6778313846	8.2255656263
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O	12.5487383090	-0.6080154890	4.2334939360
O	12.5487383090	2.6404330640	7.4819424890
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O	12.5258636973	2.5368135753	14.0536610353
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O	14.0282383090	1.3722370520	2.9652979240
O	14.0282383090	4.6206856050	6.2137464770
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Ti	16.9872383090	-0.6080154890	2.9652979240
Ti	16.9872383090	2.6404330640	6.2137464770
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O	15.4933637824	-0.6756639051	8.2131620570
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O	15.5077383090	-0.6080154890	4.2334939360
O	15.5077383090	2.6404330640	7.4819424890
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Ti	2.1922383090	5.8888816170	2.9652979240
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O	0.7127383090	5.8888816170	4.2334939360
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O	5.1328773646	13.5522408768	12.9846902033
O	5.1512383090	14.3660312630	2.9652979240
O	5.1512383090	17.6144798160	6.2137464770
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Ti	6.6307383090	15.6342272750	2.9652979240
Ti	6.6307383090	12.3857787220	6.2137464770
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Ti	6.6219066374	12.3464524490	12.6319239897
Ti	8.1102383090	12.3857787220	2.9652979240
Ti	8.1102383090	15.6342272750	6.2137464770
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O	8.0899320343	13.5564447946	12.8955721584
O	8.1102383090	14.3660312630	2.9652979240
O	8.1102383090	17.6144798160	6.2137464770
O	8.0949830934	14.3213587682	9.5654205535
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Ti	9.5968032154	15.6955499452	9.6306531564
Ti	9.5756074369	12.3315155627	12.6177494768
Ti	11.0692383090	12.3857787220	2.9652979240
Ti	11.0692383090	15.6342272750	6.2137464770
Ti	11.0804573552	12.4229269897	9.4201404305
Ti	11.0033951483	15.5510871405	12.9665874693
O	9.5897383090	12.3857787220	1.6971019120
O	9.5897383090	15.6342272750	4.9455504650
O	9.5856735905	12.3735884352	8.2535957721
O	9.5736566141	15.6817772062	11.5019653188
O	9.5897383090	12.3857787220	4.2334939360
O	9.5897383090	15.6342272750	7.4819424890
O	9.5769563529	12.3678370143	10.8186388185

O	9.5686219343	15.5018129421	14.0585756942
O	11.0692383090	16.9024232870	2.9652979240
O	11.0692383090	13.6539747350	6.2137464770
O	11.0923475649	16.8995298737	9.5052770284
O	11.0509609733	13.5447341279	12.8894387723
O	11.0692383090	14.3660312630	2.9652979240
O	11.0692383090	17.6144798160	6.2137464770
O	11.0471572352	14.3216710990	9.4760621983
O	11.0966145162	17.5711255967	12.9158544336
Ti	12.5487383090	15.6342272750	2.9652979240
Ti	12.5487383090	12.3857787220	6.2137464770
Ti	12.5698271621	15.5794476780	9.6213642461
Ti	12.5536388297	12.3279188751	12.5553148190
Ti	14.0282383090	12.3857787220	2.9652979240
Ti	14.0282383090	15.6342272750	6.2137464770
Ti	14.0532067042	12.3025970207	9.3447368893
Ti	13.9674700836	15.5472845202	12.9645873399
O	12.5487383090	12.3857787220	1.6971019120
O	12.5487383090	15.6342272750	4.9455504650
O	12.5277627790	12.3748039546	8.2154463635
O	12.5348719340	15.5047184115	11.4479324055
O	12.5487383090	12.3857787220	4.2334939360
O	12.5487383090	15.6342272750	7.4819424890
O	12.5969943334	12.3728093561	10.7571093253
O	12.5296615531	15.5062292537	14.0499367341
O	14.0282383090	16.9024232870	2.9652979240
O	14.0282383090	13.6539747350	6.2137464770
O	14.0655949229	16.8920086184	9.5598650809
O	14.0119113351	13.5417417293	12.8926499811
O	14.0282383090	14.3660312630	2.9652979240
O	14.0282383090	17.6144798160	6.2137464770
O	14.0212894760	14.3176164243	9.4655784026
O	14.0101280822	17.5440808611	12.7921820841
Ti	15.5077383090	15.6342272750	2.9652979240
Ti	15.5077383090	12.3857787220	6.2137464770
Ti	15.5306974384	15.5189490414	9.6158382332
Ti	15.5133461400	12.3242266701	12.5538341497
Ti	16.9872383090	12.3857787220	2.9652979240
Ti	16.9872383090	15.6342272750	6.2137464770
Ti	17.0205221992	12.3075491754	9.4183292590
Ti	16.9380882686	15.5557817907	12.9700633685
O	15.5077383090	12.3857787220	1.6971019120
O	15.5077383090	15.6342272750	4.9455504650
O	15.5628789794	12.3784066426	8.2163074368
O	15.5717490353	15.5007400976	11.4449047829
O	15.5077383090	12.3857787220	4.2334939360
O	15.5077383090	15.6342272750	7.4819424890
O	15.4955632501	12.3768148918	10.7503458927
O	15.4765264841	15.5910796516	14.0477758297
O	16.9872383090	16.9024232870	2.9652979240
O	16.9872383090	13.6539747350	6.2137464770
O	17.0055469294	16.9093912942	9.4888752490
O	16.9673801684	13.5397384233	12.9845383127
O	16.9872383090	14.3660312630	2.9652979240
O	16.9872383090	17.6144798160	6.2137464770
O	17.0462472253	14.3192357992	9.4719854954
O	16.9756935766	17.5650499976	12.8759620965
Au	10.1175759855	4.0775150888	19.5253004869
Au	6.8556173735	3.9181829051	16.0098822130
Au	8.3784336865	7.7852822085	18.6548597714
Au	12.0719706791	5.8539050554	15.7114208338
Au	14.1623553754	4.4951836584	16.9705302308
Au	8.9745994455	2.6716337667	17.3998323787
Au	8.5717554147	5.9789476104	20.8486423129

Au	11.1106553122	8.6887154340	18.6452875896
Au	9.8756514799	7.6641630127	16.2827356498
Au	7.5919540643	4.9197235471	18.4995149729
Au	12.5418783301	8.6165065396	16.2632201851
Au	9.4764816482	4.9671311190	15.6478733102
Au	11.3821796323	6.4348359137	20.5167419961
Au	13.1300486795	6.8041351875	18.2375022108
Au	11.5851177560	3.4225552001	17.1413938594
Au	7.2610185679	6.6982332524	16.3416228541
Au	9.6971117089	8.6124277041	21.0029624795
Au	12.8965600284	4.3453144959	19.5247026753