

**2D – 3D structural transition in sub-nanometer Pt_N clusters
supported on CeO₂(111)**

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1st June 2017

Supplementary information

Tables

Table S1. CeO₂ bulk lattice constant PBE+U calculation, as a function of the kinetic energy cutoffs and number of k-points, with U = 4.5 eV.

Table S2. Adsorption energy (E_{ads}) converge test for the supported Pt₁/CeO₂(111) adatom, as a function of the kinetic energy cutoffs and supercell size (2x2, 3x3, 4x4), including atomic thickness (O-Ce-O unit layers). Gamma point is sampled with a U = 4.5 eV.

Table S3. Bader charge transfer analysis for the putative global minima configurations of supported Pt_N/CeO₂(111) clusters reported in this work, for N = 1 to 10 atoms. Each column shows the calculated charge per Pt atom within the cluster (black colour), while the overall average charge value of the Pt_N cluster is shown in red. Valence electrons considered for the Pt atom is equal to 10e⁻.

Table S4. Calculated average bond lengths (Å), binding energies (E_{bin}) as well as total energy differences (ΔE_{Total}) between CeO₂(111) supported Pt_N clusters - as in the gas-phase - with respect to putative GM configurations of Pt_N gas-phase clusters, for N = 2 – 10.

Table S5. Calculated adhesion energies (E_{adh}) for the putative global minima configurations of CeO₂(111) supported Pt_N clusters, for N = 2 – 10.

Lattice constant a (Å)	Kinetic energy cutoff for wavefunctions and charge density (in Ry)				
k-points	25/200	30/240	35/280	40/320	45/260
4x4x4	5.434	5.515	5.519	5.507	5.505
6x6x6	5.437	5.516	5.519	5.507	5.504
8x8x8	5.436	5.515	5.519	5.507	5.505
10x10x10	-	-	-	5.507	5.504

Table S1.

E_{ads} (eV)	CeO ₂ (111) surface slab size							
Kinetic energy cutoff for wavefunctions and charge density (in Ry)	2x2 (2L)	2x2 (3L)	2x2 (4L)	3x3 (2L)	3x3 (3L)	3x3 (4L)	4x4 (2L)	4x4 (3L)
20/160	2.666	2.779	2.936	2.341	2.664	2.666	2.286	2.650
30/240				2.474	2.659	2.667	2.439	2.561
40/320				2.495	2.652	2.657	2.519	2.562

Table S2.

Bader Charge (e ⁻)	Pt ₁	Pt ₂	Pt ₃	Pt ₄	Pt ₅	Pt ₆	Pt ₇	Pt ₈	Pt ₉	Pt ₁₀
	9.833	10.063	10.038	9.966	10.051	9.887	9.938	9.938	9.949	9.947
		9.987	9.915	9.937	9.772	9.920	9.927	9.945	9.918	9.913
			10.068	9.996	9.794	9.968	9.940	9.923	9.879	9.887
				10.015	10.113	10.332	10.362	10.333	10.244	10.214
					9.974	10.033	9.954	9.906	9.940	9.939
						9.874	9.917	9.935	9.950	9.954
							9.934	9.917	9.930	9.943
								10.054	9.894	9.940
									9.915	9.962
										9.930
Average cluster charge	9.833	10.025	10.007	9.978	9.941	10.002	9.996	9.994	9.958	9.963

Table S3.

Cluster size Pt _N	Putative gas-phase GM clusters configurations		Putative supported GM clusters configurations (as in the gas-phase)		
	Average Pt-Pt bond length (Å)	Calculated binding energy, E _{bin} (eV)	Average Pt-Pt bond length (Å)	Calculated binding energy, E _{bin} (eV)	ΔE _{Total} w.r.t GM gas-phase clusters (eV)
Pt ₂	2.361	1.77	2.500	1.69	+0.15
Pt ₃	2.510	2.36	2.511	2.09	+0.83
Pt ₄	2.533	2.66	2.589	2.51	+0.61
Pt ₅	2.626	2.91	2.640	2.34	+2.82
Pt ₆	2.547	3.13	2.612	2.90	+1.39
Pt ₇	2.585	3.24	2.667	3.06	+1.31
Pt ₈	2.627	3.37	2.679	3.15	+1.77
Pt ₉	2.637	3.50	2.665	3.24	+2.37
Pt ₁₀	2.672	3.65	2.689	3.35	+3.02

Table S4.

Supported Cluster size Pt_N	Calculated adhesion energy, E_{adh} (eV)
Pt_2	6.90
Pt_3	9.18
Pt_4	11.92
Pt_5	15.18
Pt_6	12.35
Pt_7	13.91
Pt_8	15.34
Pt_9	13.45
Pt_{10}	13.22

Table S5.

DFT-based Basin Hopping Monte Carlo (BH-DFT) global optimization approach

The BH-DFT global optimization tool starts by randomly placing a Pt atom across the *xy* slab plane, at an initial height (*h*) approximately 2.0 Å away from the CeO₂(111) surface, see Figure S1. The next atom is positioned according to the spherical coordinates notation: polar and azimuthal angles (θ, ϕ) are randomly generated according to a normal distribution between 0 and 2π ; while the radial distance (*r*) value is randomly taken from a lower and upper Pt-Pt bond length range i.e. 1.50 Å to 2.50 Å, as highlighted in Figure S2. The next atom is placed at a new randomly generated (*r, θ, φ*) coordinates. Subsequent Pt atoms are placed by randomly selecting a previously generated Pt atom, which is now used as a starting point. This leads to a “pseudo” spherical 3D initial Pt_N configuration, where Pt atoms are placed at a distance no shorter than 1.20 Å. Flat (planar) structures can be enforced by constricting the *z* coordinate to a fixed distance from the substrate. The same procedure applies to Pt_N gas-phase clusters.

Once the initial gas-phase or supported Pt_N cluster has been generated, it undergoes a DFT relaxation to bring it to a local minimum. For a converged structure, a *move* factor of 0.6 Å, multiplied by a normal random distribution between (-1, 1), is applied to the cluster *xyz* coordinates. This ensures that the random displacement (or “*kick*”) displaces all Pt_N *xyz* coordinates in all directions. This move highly disrupts the Pt_N cluster, and it is the equivalent to escape from an attractive energy basin and

land in another area of the vast PES landscape at each Monte Carlo (MC) step. In case the initial structure did not SCF converged, it is once more randomly generated and subjected to a DFT relaxation. Next, the MC criterion ($e^{-\Delta E/kT}$) is used to accept/reject relaxed putative Pt_N minima configurations. We use a fictitious temperature of 2500 K to increase the probability to accept higher energy Pt_N configurations. 100 MC steps are performed for gas-phase Pt_N clusters, while between < 100 MC steps are performed for supported Pt_N clusters due to the computational intensive BH-DFT searches which now involve DFT relaxations on 81 and 144 atom surfaces, for (3x3) and (4x4) supercells respectively. BH-DFT searches are performed with a low kinetic energy cut-offs of 20/180 Ry for both wave function and charge density to allow for a rapid scan of the supported clusters PES. After BH-DFT searches, energetically stable minima configurations are further DFT relaxed using a higher wave function/charge density cut-off values (40/320 Ry).

Here, we must mention some of the current BH-DFT limitations on supported clusters. Performing BH-DFT searches from random structures on the (3x3) $CeO_2(111)$ up to size Pt_5 was already a complicated and time-consuming task. Dealing with a (4x4) surface slab extremely severed our BH-DFT searches, due to current cpu-time limitations, thus we were able only to perform BH-DFT searches up to the supported Pt_6 cluster. For supported Pt_6 up to Pt_{10} , most of the putative minima and high-energy isomers searches reported in this work were constructed following the planar (3x3) supported Pt_N cluster trends, though considering at least 3 different configurations including 3D configurations at each Pt_N cluster size.

Figures

Figure S1. Basin Hopping Monte Carlo (BH-DFT) flowchart implementation for supported $\text{Pt}_N/\text{CeO}_2(111)$ clusters, for $N = 1 - 10$. Simple random xyz moves are applied to relaxed Pt_N configurations via a “kick” factor ($0.6 \text{ \AA}$). It is multiplied by a random number generated using a normal random distribution between $(-1, 1)$ to allow atom displacements in all xyz directions.

Figure S2. Initial configurations of ceria supported Pt_N clusters. Configurations are randomly generated using spherical (r, θ, ϕ) coordinates. The first Pt atom is placed at minimum fixed height ($2 \text{ \AA}$), above the oxide surface. Then, our code randomly selects one of the previously generated Pt atoms and uses it as a pivot point to randomly generated a new (r, θ, ϕ) Pt atom.

Figure S3. Putative global minima and relevant high-energy isomers for gas-phase Pt_N clusters 2 up to 6 atoms found in our BH-DFT searches. Total energy differences, with respect to the lowest energy configuration, are shown in eV. Red dashed squares highlight other structures recently reported in the literature [1].

Figure S4. Putative global minima and relevant high-energy isomers for gas-phase Pt_N clusters 7 up to 10 atoms. Total energy differences, with respect to the lowest energy configuration, are shown in eV. Red dashed squares highlight some structures recently reported in the literature, although not found in our DFT-BH searches as global minima (see: Demiroglu, I.; Yao, K.; Hussein, H.A.; Johnston, R.L.; *J. Phys. Chem. C* Article ASAP (2016) (**DOI:** 10.1021/acs.jpcc.6b11329))

Figure S5. Projected density of states (PDOS) plots comparison between the putative global minima configurations of gas-phase Pt_N (*left*) and the supported (3x3) $\text{Pt}_N/\text{CeO}_2(111)$ configurations (*right*), for $N = 1 - 5$. The oxide O(*p*), Ce (*f*, *d*, *s*) and the cluster Pt (*d*, *s*) electronic states are shown. The vertical (black) line indicates the position of the Fermi level.

Figure S6. Projected density of states (PDOS) plots for the putative global minima configurations of gas-phase Pt_N (*left*) and the supported (4x4) $\text{Pt}_N/\text{CeO}_2(111)$ configurations (*right*), for $N = 6 - 10$. The oxide O(*p*), Ce (*f*, *d*, *s*) and the cluster Pt (*d*, *s*) electronic states are shown. The vertical (black) line indicates the position of the Fermi level.

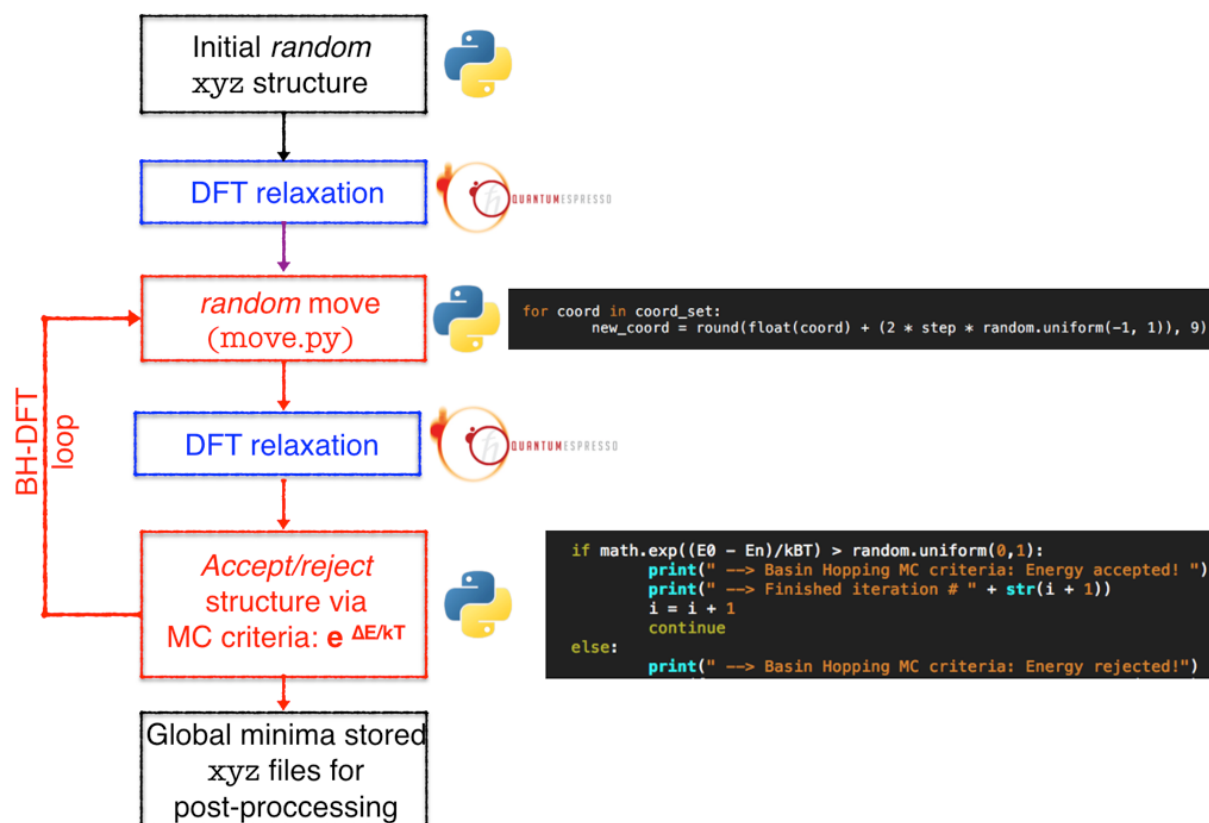


Figure S1.

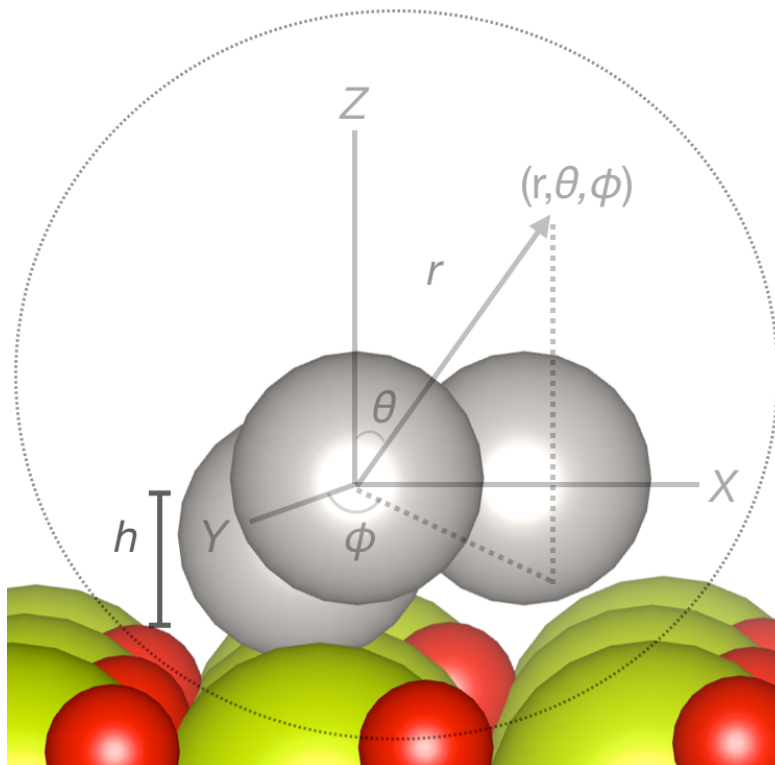


Figure S2.

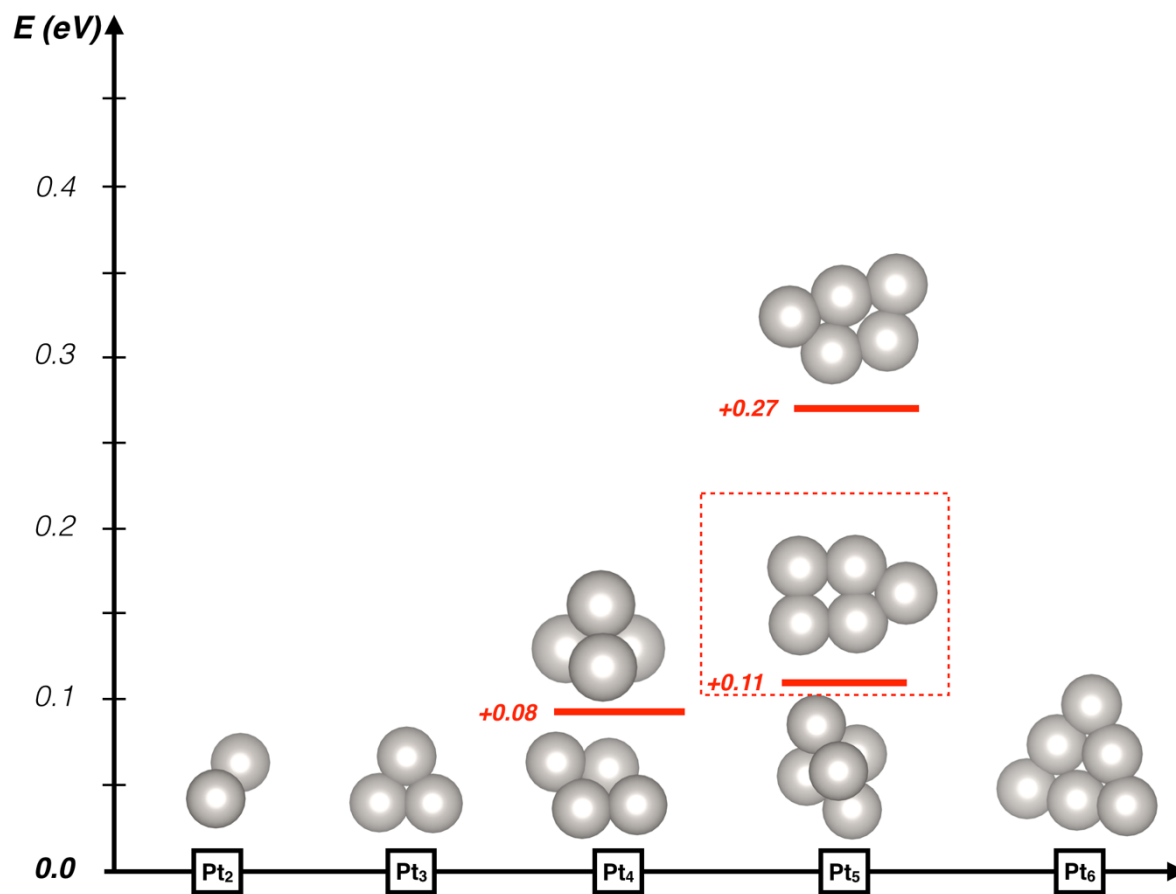


Figure S3.

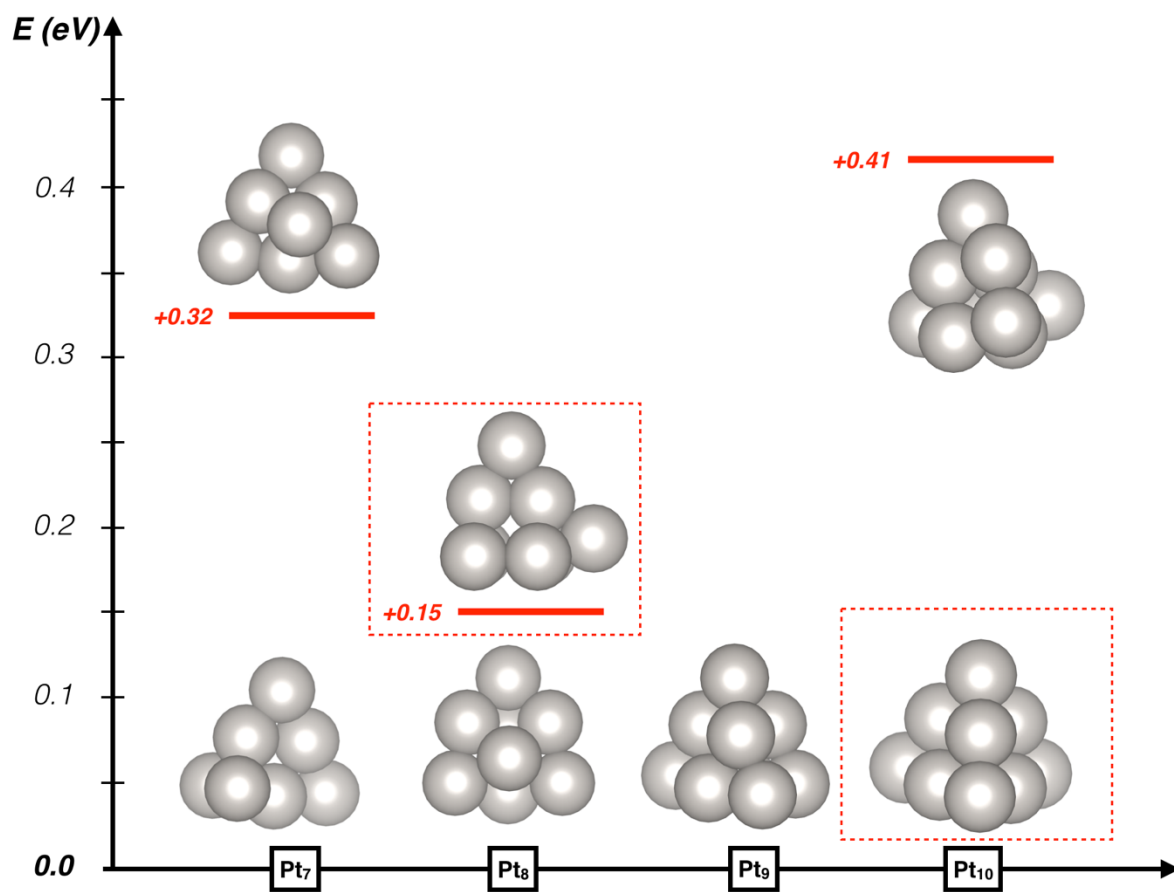
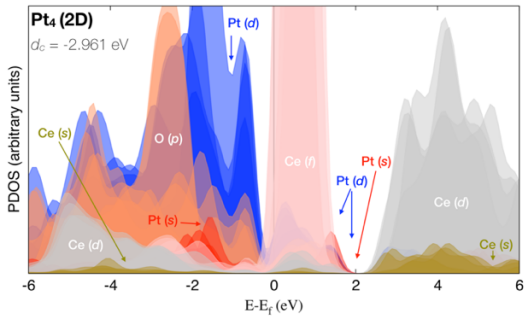
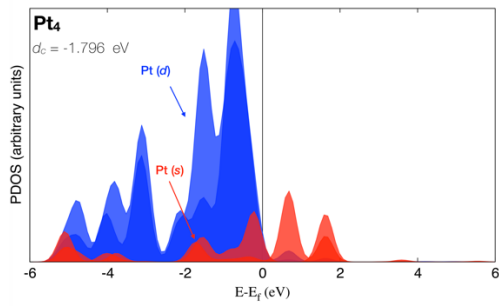
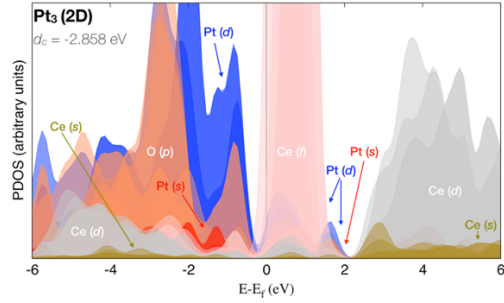
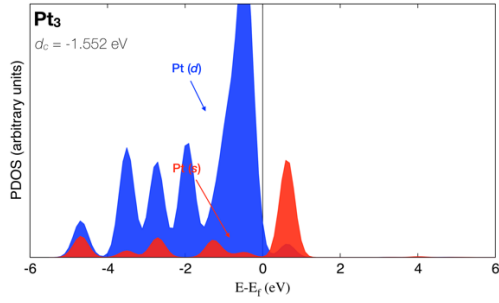
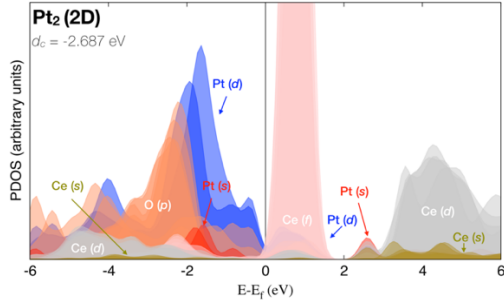
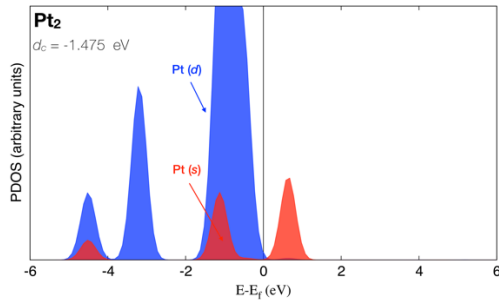
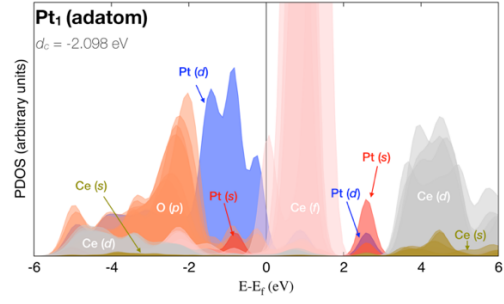
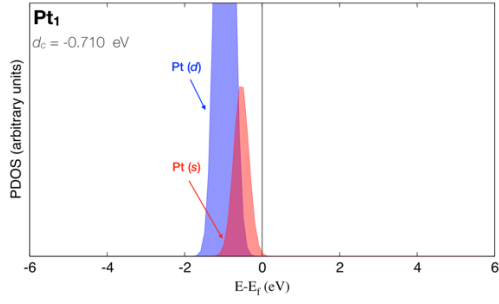
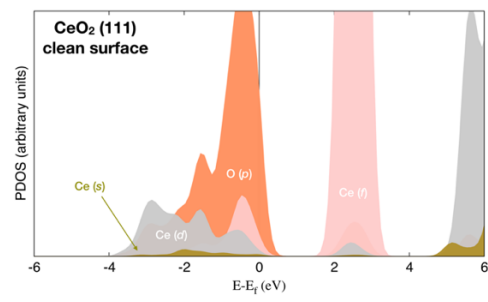


Figure S4.



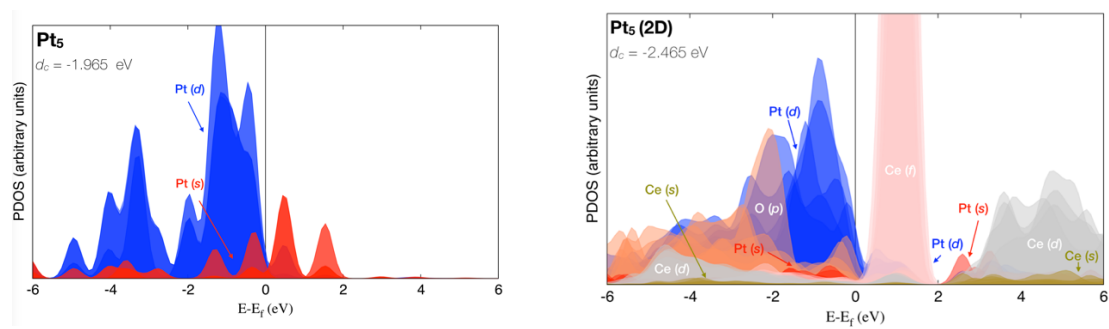
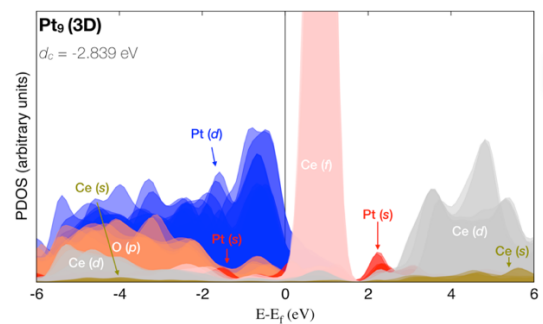
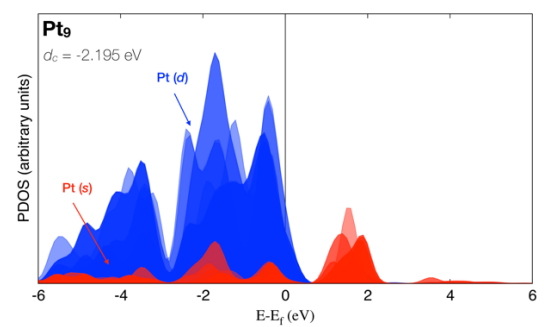
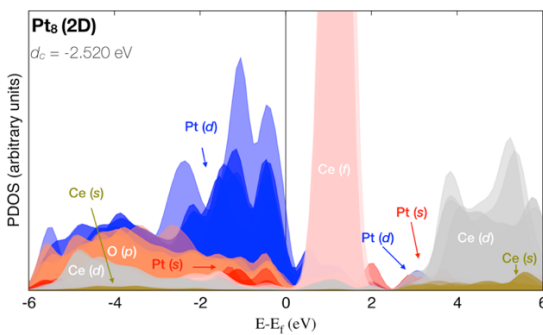
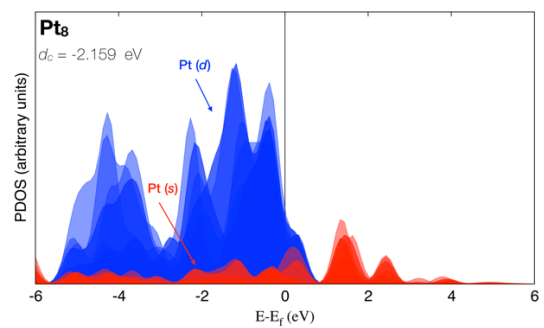
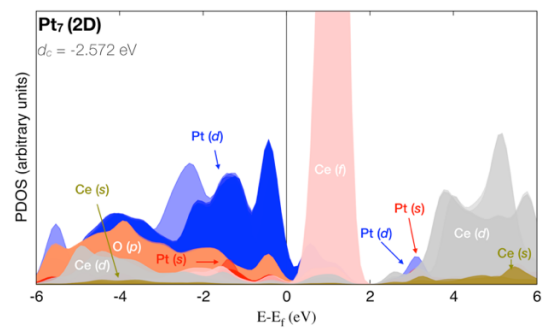
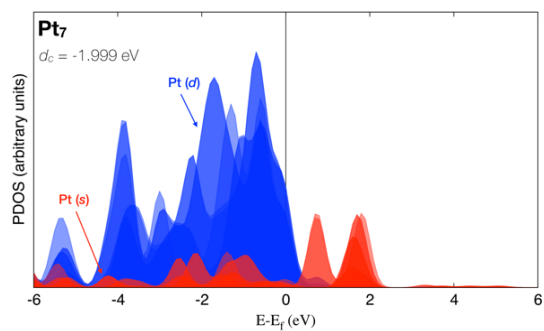
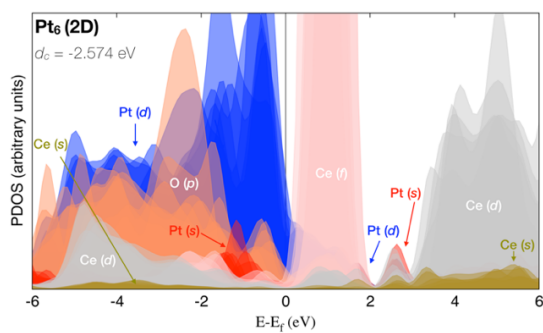
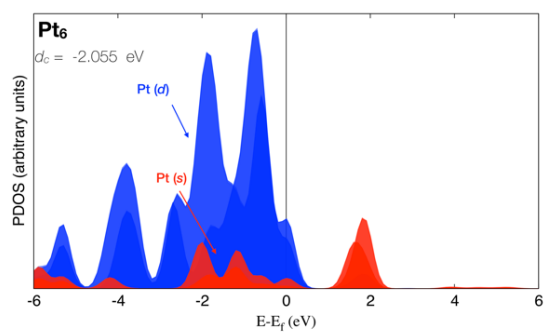


Figure S5.



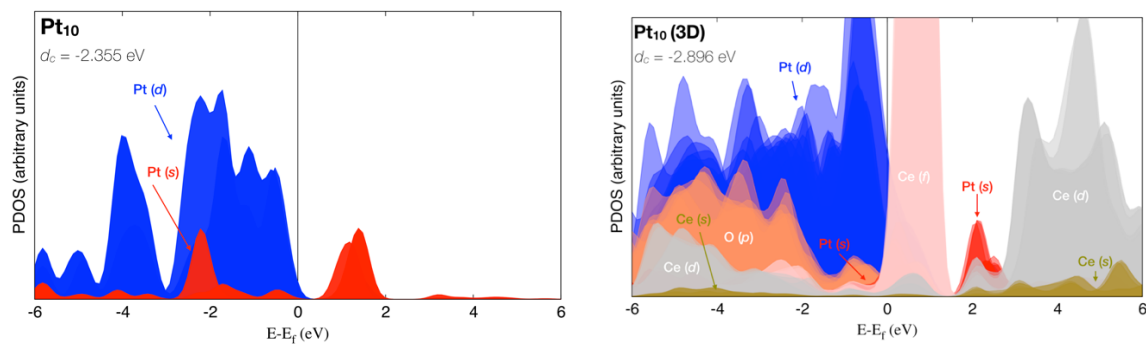


Figure S6.

Gas-phase Pt_N clusters – xyz coordinates

GM – Global minimum

Iso – Low-lying energy Isomer

Pt₂ - GM (0.0 eV)

2

Pt	1.394139795	6.248816477	3.931587905
Pt	0.246540193	4.559125941	5.116125357

Pt₃ - GM (0.0 eV)

3

Pt	7.374835935	4.199665593	7.649287920
Pt	7.654097847	2.440409841	9.417152069
Pt	9.323298433	2.620176526	7.552580019

Pt₄ - GM “butterfly” (0.0 eV)

4

Pt	3.311704959	3.409589474	6.719802944
Pt	1.684022326	5.563758238	3.412948363
Pt	3.719311159	5.001814822	4.798576458
Pt	1.699010785	3.434152629	4.775654098

Pt₄ - Iso1 “Td” (+0.08 eV)

4

Pt	7.120671066	7.325557985	2.589949642
Pt	7.233215380	9.248082884	4.360059214
Pt	5.776707391	7.122056560	4.824993026
Pt	5.031484164	8.848450571	3.002429118

Pt₅ - GM “bi-tetrahedron” (0.0 eV)

5

Pt	7.137581796	7.305433025	2.565178681
Pt	7.210141262	9.247386722	4.364961702
Pt	5.777429276	7.141254282	4.822812231
Pt	4.873391272	9.503641799	5.583911752
Pt	5.036925974	8.850073494	3.024477919

Pt₅ - Iso1 “square” (+0.11 eV)

5

Pt	6.026210120	7.747400833	2.501043441
Pt	7.403555282	5.820017057	3.351192625
Pt	5.776510489	7.050543281	4.831898387
Pt	4.246119161	8.961583645	5.266051792
Pt	4.502333073	9.668346968	2.888199559

Pt₅ - Iso2 “W-type” (+0.27 eV)

5

Pt	6.715660454	6.887962781	2.290377954
Pt	7.306988308	5.302497479	4.147303398
Pt	5.777891357	7.079441304	4.972243629
Pt	4.184657498	8.951718077	5.382248170
Pt	5.133416125	8.705855181	3.080869312

Pt₆ - GM “2D triangle” (0.0 eV)

6

Pt	4.774962837	9.479506542	2.245718326
Pt	2.020494924	5.392067849	2.336601227
Pt	1.547098785	7.082881345	4.070147930
Pt	3.050954197	9.331022632	4.003448492
Pt	1.286641834	8.932071992	5.680665297
Pt	3.448446599	7.397831640	2.159026287

Pt₇ - GM (0.0 eV)

7

Pt	4.852727718	7.829704838	9.480684182
Pt	2.792922487	6.094569666	9.739558107
Pt	0.639236025	7.352544659	9.046153822
Pt	4.916574706	5.895459603	11.018640204
Pt	2.776306191	8.045291017	7.757370902
Pt	1.703044663	5.718256319	7.411024403
Pt	4.636565727	9.687470097	7.860322944

Pt₇ - Iso1 (+0.32 eV)

7

Pt	4.836731715	8.017000149	9.640819127
Pt	2.622637458	6.275279714	9.859664209
Pt	0.795062872	6.787962109	8.218989155
Pt	4.954726711	5.722597966	10.803282488
Pt	2.886470098	7.960458004	7.592455017
Pt	4.537107970	5.918798124	8.209768356
Pt	4.568791608	9.762262335	7.856443806

Pt₈ - GM (0.0 eV)

8

Pt	3.655996655	7.356516786	6.278586018
Pt	3.782986159	10.442230651	8.397982088
Pt	4.814005972	9.707175888	6.185095786
Pt	2.292287828	9.551566801	5.878234667
Pt	1.270122370	10.641190876	9.231014040
Pt	2.205322567	8.449443839	8.170807243
Pt	4.644505762	12.262233437	6.667935546
Pt	2.090046698	11.845646863	7.057099807

Pt₈ - Iso1 (+0.15 eV)

8

Pt	8.362426064	6.757754854	8.933364893
Pt	5.876559804	6.256436183	8.398424188
Pt	8.210280370	8.924368799	7.592122168
Pt	5.721677703	8.417447509	7.080885858
Pt	3.882359820	6.590258931	6.739253865
Pt	8.762572055	6.702750317	6.363731805
Pt	6.358650821	6.249471564	5.891642485
Pt	8.126773363	5.402911842	4.301874737

Pt₉ - GM (0.0 eV)

9

Pt	1.592548204	5.017323823	5.522182635
Pt	2.844030254	9.285890022	4.535576824
Pt	4.676614241	4.721634531	3.587579675
Pt	2.195468214	5.014860066	3.060378622
Pt	3.288915318	7.145818809	5.943706814
Pt	3.889352189	7.149916345	3.478932377
Pt	1.184208005	7.406545477	4.120480955
Pt	4.053708738	4.712796020	6.134687428
Pt	-0.284531515	5.368336259	3.749702918

Pt₁₀ - GM "Td" (0.0 eV)

10

Pt	8.132673981	7.340681536	8.141934007
Pt	5.939748521	6.020213023	8.062640766
Pt	3.777643004	4.708315882	7.665752626
Pt	8.007333160	5.627661824	6.244483538
Pt	6.568818548	8.011516203	6.225727575
Pt	5.637401297	4.197344413	5.981479152
Pt	4.196724966	6.578651650	5.965898187
Pt	7.576977092	3.996316271	4.319024442
Pt	4.933893397	8.369722325	4.286761291
Pt	6.269086035	6.190176873	4.146798417

Pt₁₀ - Iso1 (+0.41 eV)

10

Pt	6.818947011	6.145009373	4.152181471
Pt	6.000927630	6.453517796	6.624696407
Pt	6.875170962	9.568365217	3.170739808
Pt	8.710264840	6.546616286	2.500373802
Pt	7.365500392	8.287332890	5.349252853
Pt	6.318556141	7.384904204	1.899846004
Pt	9.236158768	8.713429118	3.721949941
Pt	8.255299867	10.730192342	5.079811169
Pt	8.538836822	6.113881816	6.067350684
Pt	10.481549980	6.515478489	4.408200437

Supported Pt_N/ CeO₂(111) clusters – xyz coordinates

NOTE: 0's on the right indicate those Ce and O atoms kept fixed during Quantum Espresso DFT relaxations.

Pt₁/ CeO₂(111) - GM (0.0 eV)

82

O	0.003508277	-0.005979152	3.152805452			
O	-1.953936618	3.371371166	3.170770331			
O	-3.884927170	6.738318510	3.151480024			
O	3.899266267	-0.012640614	3.147555826			
O	1.943058788	3.351135291	3.158128149			
O	-0.006130709	6.745128118	3.160202366			
O	7.795974166	0.018612144	3.163942688			
O	5.865218651	3.356320930	3.137553553			
O	3.903234301	6.743997008	3.162346131			
O	0.099610291	2.252579189	6.407654099			
O	-1.955195432	5.608935400	6.354246819			
O	-3.916530908	8.977280573	6.374468347			
O	3.813222559	2.194567017	6.371139038			
O	2.018843615	5.612327404	6.231950837			
O	-0.000048436	9.004405314	6.354868038			
O	7.827773984	2.240466877	6.309775010			
O	5.739219574	5.677296480	6.420647869			
O	3.935311718	8.966868630	6.368763616			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	0.022391497	-0.002652688	7.993521482			
O	-1.953597838	3.357436839	7.939109776			
O	-3.907943868	6.725733048	7.952021149			
O	3.864831676	-0.028224321	7.960275451			
O	1.827460910	3.555557133	8.278059287			
O	-0.056934431	6.770715687	7.923606548			
O	7.788071475	0.051581234	7.934847686			

O	5.902177704	3.293567530	7.868797591			
O	3.729404291	7.138796529	8.421910481			
O	1.947205469	1.083899255	4.782523661			
O	-0.013995912	4.484522688	4.798817886			
O	-1.947914135	7.864926575	4.797037809			
O	5.829549768	1.132457507	4.793315295			
O	3.950955877	4.426641904	4.708905144			
O	1.950616811	7.905636027	4.779188701			
O	9.781451763	1.124061602	4.817222967			
O	7.750239746	4.522111316	4.813501668			
O	5.853982959	7.858645584	4.793887634			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.937308626	1.038001570	7.182223810			
Ce	0.021892045	4.535375414	7.198202186			
Ce	-1.955248288	7.853969507	7.157035742			
Ce	5.870621076	1.092366136	7.141134815			
Ce	3.978830497	4.350428123	7.015505763			
Ce	1.940565348	7.899472958	7.197497690			
Ce	9.750139118	1.144170092	7.162125765			
Ce	7.808172439	4.487240900	7.150483357			
Ce	5.835645126	7.893961817	7.216005852			
Ce	0.018850074	2.247028742	3.988749077			
Ce	-1.936581700	5.615486285	3.979435736			
Ce	-3.897961356	8.977146938	3.969745862			
Ce	3.891726956	2.212450210	3.937754550			
Ce	1.944586950	5.623484504	3.970202868			
Ce	0.015338360	8.983584658	3.974946050			
Ce	7.792999202	2.250023523	3.966723783			
Ce	5.844655566	5.629676542	3.959020703			
Ce	3.904045522	8.986096809	3.982855461			
Pt	2.664177522	5.425885495	8.986953373			

Pt₂/ CeO₂(111) - GM (0.0 eV)

83

O	-0.016876755	-0.000499077	3.182338747			
O	-1.942417116	3.360540465	3.151501152			
O	-3.891960845	6.748109309	3.149086003			
O	3.893261495	-0.005764861	3.150396205			
O	1.944659267	3.372823636	3.167793869			
O	0.001226536	6.739083411	3.150264583			
O	7.780830583	-0.012153784	3.176882619			
O	5.844669601	3.363444561	3.174305080			
O	3.892329903	6.761486818	3.144435579			
O	0.039808296	2.219543312	6.294989980			
O	-1.920058797	5.626710920	6.387871647			
O	-3.904991296	9.007920079	6.318979096			
O	3.881059772	2.344634728	6.380612494			
O	1.933939441	5.495957359	6.405704045			
O	0.003379507	8.948784135	6.318509192			
O	7.635831465	2.290986459	6.455871030			
O	5.914573790	5.548187598	6.404355827			
O	3.888208641	9.030861674	6.314353738			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.018433607	-0.029701228	7.936579445			
O	-1.841306705	3.315548802	7.885008383			
O	-3.846761393	6.865556458	7.955950384			
O	3.897873337	-0.058396814	7.909354739			
O	1.377019200	2.970191810	8.432832109			
O	0.023319122	6.751602062	7.961495346			
O	7.766412760	-0.071234688	7.931226672			
O	7.301118759	3.850277510	9.291388417			
O	3.912359556	6.837475239	7.864492607			
O	1.976985959	1.118572121	4.779886875			
O	-0.014551465	4.500224574	4.781610103			
O	-1.954787132	7.854569662	4.778682934			
O	5.810269064	1.094672182	4.787350488			
O	3.914046812	4.553221626	4.712620403			

O	1.947445220	7.809588099	4.812115215			
O	9.674728167	1.168308908	4.827070893			
O	7.823763636	4.496466701	4.760344797			
O	5.836491617	7.832442432	4.803839039			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.923711944	1.065645295	7.163507477			
Ce	-0.047995571	4.477860332	7.168492003			
Ce	-1.942480478	7.850790869	7.152837487			
Ce	5.815741405	0.978145808	7.129582427			
Ce	3.945559499	4.680128144	7.028988451			
Ce	1.932763108	7.858299717	7.159416060			
Ce	9.715327644	1.115049512	7.147216484			
Ce	7.894856072	4.554143083	7.301035608			
Ce	5.866374900	7.905771686	7.145010866			
Ce	-0.002906095	2.249993636	3.972555751			
Ce	-1.951157736	5.602629969	3.968485333			
Ce	-3.887669613	8.993823746	3.961690716			
Ce	3.888134303	2.247618587	3.988847464			
Ce	1.934896703	5.612252124	3.948186051			
Ce	-0.007491346	8.973648885	3.946796665			
Ce	7.767731405	2.268666211	4.003869691			
Ce	5.877585499	5.618892712	3.954185469			
Ce	3.881111950	8.981454464	3.971586519			
Pt	5.498088865	3.233381184	9.080283415			
Pt	3.027612993	3.512233284	9.344439388			

Pt₂/ CeO₂(111) – “Iso1_2D” (+0.25 eV)

83

O	0.019580959	-0.024436957	3.177757440			
O	-1.930726856	3.373561441	3.147712756			
O	-3.886952919	6.752089206	3.153627064			
O	3.901002494	0.002915271	3.170206892			
O	1.944985582	3.367351885	3.152828052			
O	0.006305028	6.750341940	3.150729296			
O	7.808861381	-0.004744474	3.141790117			
O	5.848064167	3.385385854	3.171687649			
O	3.875368285	6.756003801	3.166118857			
O	0.022239640	2.213146877	6.331729876			
O	-1.898883682	5.648237774	6.347066264			
O	-3.914494480	8.972607218	6.292684064			
O	4.030774498	2.272134096	6.353518733			
O	1.907006089	5.674698047	6.310557964			
O	-0.104636619	9.107002094	6.477018275			
O	7.876064571	2.300585701	6.287610924			
O	5.806109103	5.448826360	6.445754706			
O	3.927066202	8.978111876	6.317439703			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.020212281	-0.020546665	7.944749389			
O	-1.841250745	3.399322848	7.940165580			
O	-3.909081807	6.705657142	7.926706151			
O	3.184146827	-0.523500958	8.498126778			
O	1.875038217	3.433055388	7.905251710			
O	0.028501237	6.769131711	7.973721951			
O	7.896276155	0.016004470	7.907599556			
O	6.653896087	3.153751890	8.472016213			
O	3.842499393	6.793420343	7.929029047			
O	1.985132448	1.135253446	4.807678257			
O	0.001889610	4.486777638	4.773869936			
O	-1.916599709	7.866665682	4.790110589			
O	5.916477354	1.126097868	4.741692898			
O	3.848056812	4.515067780	4.752650836			

O	1.892900454	7.920637751	4.822495555			
O	9.760385679	1.115257786	4.765238764			
O	7.818029172	4.540001856	4.768626381			
O	5.836571199	7.779863006	4.821838817			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.898018657	1.074335748	7.179758012			
Ce	0.008066657	4.510366887	7.148566731			
Ce	-1.971195581	7.831175443	7.209744313			
Ce	6.072591057	1.183291299	7.105314759			
Ce	3.729633721	4.559752872	7.096078144			
Ce	1.927110705	7.898558065	7.161532767			
Ce	9.806329299	1.122344503	7.125927944			
Ce	7.926582205	4.547984834	7.140705816			
Ce	5.824916242	7.832071549	7.145827023			
Ce	0.028420834	2.241153208	3.963681410			
Ce	-1.933626769	5.635337065	3.949088238			
Ce	-3.876148363	8.978736934	3.973303858			
Ce	3.910830801	2.247747502	3.994154938			
Ce	1.927606915	5.628123027	3.939688704			
Ce	-0.007042078	9.009494987	3.976752621			
Ce	7.824270928	2.257936156	3.931269010			
Ce	5.842136608	5.598709576	3.984253199			
Ce	3.894652734	8.984345024	3.967566190			
Pt	5.006573915	3.445324246	9.410275407			
Pt	4.168117447	1.076779213	9.141831400			

Pt₃/ CeO₂(111) – GM (0.00 eV)

84

O	-0.017238857	-0.006888713	3.162083822			
O	-1.954002265	3.378855797	3.140895407			
O	-3.879589637	6.732687098	3.144104677			
O	3.917580029	-0.006041757	3.157405440			
O	1.957003242	3.392710143	3.161325069			
O	0.027013795	6.761038078	3.179836520			
O	7.791355979	0.004151758	3.174952876			
O	5.848379884	3.374937191	3.148005050			
O	3.905653857	6.744742879	3.168836823			
O	0.040661096	2.266834589	6.342595650			
O	-1.918788080	5.638103103	6.330428983			
O	-3.850821580	9.038264217	6.427649120			
O	3.811350513	2.235169865	6.356799635			
O	1.937558933	5.572037690	6.285929626			
O	0.037041047	8.987412284	6.280723389			
O	7.767460010	2.267915887	6.353696283			
O	5.858232311	5.601058178	6.380707176			
O	4.048285701	9.098752650	6.432485949			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.412517942	-1.450760544	9.211159501			
O	-1.977039454	3.418400313	7.927607655			
O	-3.801171262	6.651507459	7.975728613			
O	4.751749104	-0.555487217	8.516334960			
O	1.874281178	4.042180456	8.411160093			
O	0.054717258	6.727700432	7.908743340			
O	7.809088119	0.030945193	7.916143667			
O	5.846383330	3.377480003	7.951410294			
O	3.825203458	6.663711715	7.864100074			
O	1.937653405	1.107486146	4.626137538			
O	-0.020396426	4.494169604	4.755940846			
O	-1.955732981	7.866953981	4.791968352			
O	5.833876731	1.155804421	4.806741882			
O	3.936168139	4.488823588	4.794494186			

O	2.038197551	7.888009144	4.841214853			
O	9.720851911	1.171359136	4.785068259			
O	7.795173254	4.505024807	4.786276624			
O	5.882459443	7.846532256	4.784465383			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.912834036	1.104451755	6.881015638			
Ce	-0.045353666	4.571188270	7.118624755			
Ce	-1.864084323	7.799542887	7.208658120			
Ce	5.897010501	1.105707056	7.214222572			
Ce	3.946523660	4.516665423	7.158368666			
Ce	1.993584548	7.869371789	7.141668205			
Ce	9.623726619	1.220388144	7.141805898			
Ce	7.784818439	4.509697331	7.160604693			
Ce	5.875577834	7.754148072	7.289098193			
Ce	-0.023442607	2.273882738	3.926420099			
Ce	-1.936291471	5.632776485	3.957243984			
Ce	-3.878321634	8.944739387	3.949694232			
Ce	3.922060528	2.258178893	3.943644893			
Ce	1.968546016	5.622617496	3.968247398			
Ce	0.014775129	9.003450286	3.972010364			
Ce	7.775335110	2.253302958	3.956415507			
Ce	5.849265256	5.629078306	3.971392046			
Ce	3.938512440	8.999636913	4.003239238			
Pt	3.354656946	0.707765452	9.121675005			
Pt	1.529105034	2.421473923	9.428786076			
Pt	0.103873849	0.399717620	9.077656443			

Pt₃/ CeO₂(111) – “Iso1_2D” (+0.43 eV)

84

O	-0.008619992	0.005213359	3.161869180			
O	-1.952271527	3.379955054	3.160529996			
O	-3.886753192	6.753896951	3.156819914			
O	3.914116513	0.007158484	3.159476444			
O	1.954359424	3.409122781	3.175096639			
O	-0.012467131	6.754155969	3.168053606			
O	7.790674286	0.013725790	3.159720806			
O	5.852231002	3.382182877	3.158407626			
O	3.911790079	6.754226289	3.168306151			
O	-0.011057827	2.240067690	6.283815343			
O	-1.982495221	5.684927705	6.321146278			
O	-3.892232059	9.107818655	6.469559658			
O	3.939206927	2.254441468	6.288232372			
O	1.946492215	5.708113364	6.290242036			
O	0.034918143	8.962015905	6.336536042			
O	7.797482988	2.265226423	6.383750563			
O	5.897851174	5.683601478	6.332172114			
O	3.876257195	8.957604579	6.330364889			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.545577786	-0.310462644	8.348024626			
O	-1.977998374	3.484282235	7.940104442			
O	-3.871113878	6.768774924	7.993636742			
O	4.391315137	-0.241923467	8.287139274			
O	1.956066864	3.700971027	7.732557811			
O	-0.032918108	6.712727696	7.971940235			
O	7.792618869	0.009102861	7.976907678			
O	5.898496879	3.480691244	7.949425093			
O	3.938383499	6.700274297	7.972661857			
O	1.960605306	1.141355582	4.646638474			
O	-0.037596588	4.526126313	4.784313712			
O	-1.977376502	7.905059270	4.813712719			
O	5.875351615	1.127796513	4.800685933			
O	3.944486197	4.533179015	4.793793916			

O	1.949354554	7.892128528	4.763597873			
O	9.711903799	1.124278275	4.801163732			
O	7.789829632	4.503839540	4.785376990			
O	5.884123483	7.899749995	4.811751227			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.972017208	1.234224383	6.887751784			
Ce	-0.142175761	4.581541723	7.087195232			
Ce	-1.925921583	7.857936348	7.198771450			
Ce	5.919642366	1.133905766	7.190171269			
Ce	4.057361982	4.578329057	7.099420819			
Ce	1.952139673	7.865645132	7.129089416			
Ce	9.673068215	1.120183275	7.191277060			
Ce	7.798929097	4.532478163	7.165823731			
Ce	5.832302023	7.852044613	7.206637868			
Ce	-0.031093687	2.267504080	3.937841658			
Ce	-1.955571119	5.644752633	3.946546526			
Ce	-3.886297225	8.989578515	3.959519109			
Ce	3.940468937	2.272190564	3.933700719			
Ce	1.951360757	5.643848823	3.970344034			
Ce	0.007765237	9.003976847	3.976720558			
Ce	7.792610486	2.246480451	3.979823079			
Ce	5.858954360	5.646570225	3.951278920			
Ce	3.896979016	9.001730727	3.975372075			
Pt	3.350988860	1.223473792	9.186669168			
Pt	1.863705282	3.329617014	9.582572247			
Pt	0.499816592	1.182970498	9.160314421			

Pt₄/ CeO₂(111) – GM (0.0 eV)

85

O	0.003345917	-0.002611268	3.155441097			
O	-1.970065963	3.345538350	3.173967203			
O	-3.876434378	6.730270089	3.145957067			
O	3.896904443	-0.001175060	3.149302989			
O	1.932123846	3.344411872	3.147024522			
O	-0.019463859	6.746012721	3.153829171			
O	7.763337576	0.021792916	3.165267748			
O	5.872301486	3.358200619	3.189559458			
O	3.893781395	6.768713234	3.147636743			
O	0.011881276	2.223287967	6.247509279			
O	-1.772154723	5.637317758	6.478864241			
O	-3.883889289	8.975339666	6.441016341			
O	3.849458309	2.404024080	6.391912189			
O	1.886972930	5.640573716	6.268779854			
O	-0.019262280	8.910201155	6.423845120			
O	7.761250965	2.261602755	6.302993551			
O	5.771138218	5.593654309	6.377493661			
O	3.891788587	8.817399200	6.396681593			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.043015169	0.059418455	7.884863423			
O	-1.936572251	3.278595956	7.918996111			
O	-3.848447105	6.628706040	7.954776240			
O	3.889178416	0.120967276	7.954609373			
O	1.226301031	2.764639518	8.544643049			
O	-0.824996425	7.451080902	9.056349301			
O	7.797579119	0.026678652	7.892037468			
O	6.434799001	3.047680842	8.428866460			
O	5.112595941	7.536364151	9.250348269			
O	1.986055558	1.086309036	4.792965476			
O	-0.023036621	4.461144668	4.735432803			
O	-1.966076376	7.859862756	4.781536825			
O	5.779130877	1.091864745	4.854819261			
O	3.878380824	4.524384151	4.598540802			

O	1.917685373	7.903566616	4.725824559			
O	9.720321085	1.048664080	4.818743626			
O	7.833228844	4.560974689	4.852321060			
O	5.879511438	7.858557698	4.755072910			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.917927967	1.054048802	7.194990280			
Ce	-0.079231705	4.294328587	7.121825752			
Ce	-2.018050738	7.913098688	7.312729088			
Ce	5.834037041	1.119327035	7.224793083			
Ce	3.847012483	4.600168262	6.840422170			
Ce	1.916569564	8.023005519	7.047341982			
Ce	9.735632724	1.079108806	7.140041385			
Ce	7.872934964	4.496047315	7.211248928			
Ce	5.927595819	7.881169257	7.314714633			
Ce	-0.000428439	2.222917104	3.931361556			
Ce	-1.936754426	5.624395513	3.992848826			
Ce	-3.884768755	8.970497174	3.982276775			
Ce	3.883843832	2.221860950	3.955827000			
Ce	1.896137881	5.630384985	3.912599872			
Ce	-0.034405946	8.995360017	3.968060621			
Ce	7.778837400	2.237702656	3.981257675			
Ce	5.881431753	5.652451308	3.946320097			
Ce	3.911047273	8.965860649	3.955748099			
Pt	4.850105587	3.996644264	9.197465675			
Pt	2.280694827	4.292081386	9.242095422			
Pt	3.378380373	6.640942190	9.185383003			
Pt	0.769526971	6.344388105	9.165142303			

Pt₄/ CeO₂(111) – “Iso1_2D” (+0.19 eV)

85

O	0.001827250	-0.011046423	3.165044637			
O	-1.962520372	3.375557137	3.158987336			
O	-3.877641835	6.744576872	3.151439606			
O	3.896797086	-0.021462494	3.150522615			
O	1.927671271	3.351146342	3.153394905			
O	-0.017715677	6.744478059	3.158131009			
O	7.776534716	0.012976959	3.169432330			
O	5.884811770	3.380817606	3.173801553			
O	3.901687501	6.768214634	3.153714443			
O	0.054477967	2.207740426	6.277461895			
O	-1.776866476	5.655561411	6.556434917			
O	-3.886014013	8.970813350	6.400710134			
O	3.874997363	2.336923237	6.374347328			
O	1.936043420	5.576370064	6.304169400			
O	0.009161322	9.022605104	6.330962847			
O	7.729758393	2.282936690	6.286446507			
O	5.782181925	5.572627633	6.391414584			
O	3.876988137	8.981681633	6.267018315			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.031480959	-0.050770882	7.891757622			
O	-1.929316790	3.263832841	7.897212274			
O	-3.892911891	6.750668454	7.984577654			
O	3.915628530	0.041311251	7.959868850			
O	1.136235434	2.498796200	8.706116737			
O	-0.131346602	7.538837999	8.541202731			
O	7.787324868	0.086685841	7.904326737			
O	6.688294571	3.021348094	8.563631984			
O	3.847869580	7.849681687	8.565936171			
O	1.986679858	1.083732923	4.776643879			
O	-0.033120293	4.471719447	4.768290088			
O	-1.954346977	7.845524570	4.825439885			
O	5.796259061	1.128425046	4.793294633			
O	3.896201778	4.504789845	4.590584882			

O	1.921283507	7.863060240	4.776055551			
O	9.725592941	1.137648900	4.791228907			
O	7.853482436	4.585019545	4.865523728			
O	5.870620956	7.845112488	4.813547568			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.933762602	1.002465985	7.200208990			
Ce	-0.060004803	4.273658892	7.152731744			
Ce	-1.953932147	7.927092850	7.251997726			
Ce	5.868766285	1.100305248	7.158543824			
Ce	3.856537186	4.531424689	6.823107127			
Ce	1.920635606	8.031809791	7.220057526			
Ce	9.722817750	1.087295995	7.115393296			
Ce	7.887130261	4.532888289	7.234929357			
Ce	5.850897529	7.921082474	7.217522693			
Ce	0.003830795	2.231868458	3.935429501			
Ce	-1.929371371	5.627618767	3.992653755			
Ce	-3.883709424	8.978072879	3.977254923			
Ce	3.886136044	2.208644607	3.934608777			
Ce	1.905192974	5.644105779	3.934933738			
Ce	0.002767745	8.989829159	3.974143145			
Ce	7.785792449	2.261870233	3.970380003			
Ce	5.883894536	5.649164498	3.944807686			
Ce	3.882355960	8.980002609	3.954763866			
Pt	4.959022999	3.608619372	9.260925578			
Pt	2.404612957	3.877778496	9.252565722			
Pt	3.972023049	5.966996384	9.200789868			
Pt	0.989790651	5.999173425	9.145081947			

Pt₄/ CeO₂(111) – “Iso2_3D” (+0.57 eV)

85

O	0.001878975	-0.003338539	3.133613075			
O	-1.962633979	3.356876640	3.187159249			
O	-3.874571434	6.727841591	3.147565915			
O	3.920288325	0.004980092	3.139257095			
O	1.959206581	3.351559661	3.161524924			
O	0.003693338	6.748930421	3.157910299			
O	7.760126585	0.019357862	3.169661930			
O	5.878172738	3.353787140	3.189117684			
O	3.902962956	6.736349563	3.165121470			
O	-0.016775308	2.251104152	6.206260609			
O	-1.740326800	5.650187245	6.440250514			
O	-3.865724549	8.948135618	6.438476054			
O	3.777597351	2.315232065	6.374480488			
O	1.957122234	5.595733016	6.382791631			
O	0.030631058	8.872913245	6.420171890			
O	7.792647755	2.252624703	6.358431596			
O	5.749262473	5.687854666	6.388968397			
O	3.872823198	8.822228666	6.437634084			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.086137834	0.090691525	7.859403692			
O	-1.909332351	3.324333174	7.951161790			
O	-3.819994486	6.544496432	7.950120463			
O	3.953589064	0.104702955	7.933136927			
O	1.269828885	2.625043670	8.436801661			
O	-0.964627720	7.498289685	9.076349620			
O	7.776318642	0.024293419	7.950941758			
O	5.839056580	3.379183464	7.964421393			
O	5.209497045	7.563448492	9.194073828			
O	1.957467933	1.060824953	4.760453035			
O	0.020313130	4.490798339	4.743889393			
O	-1.943888861	7.868997634	4.779781745			
O	5.803603777	1.097555902	4.882025083			
O	3.933186265	4.479962115	4.753729704			

O	1.951930805	7.871583755	4.769268516			
O	9.717682877	1.035550507	4.829607534			
O	7.822826846	4.557978104	4.886031097			
O	5.864016539	7.883800047	4.751145146			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.915025781	1.025024489	7.146818385			
Ce	-0.077533601	4.289794932	7.114916787			
Ce	-1.974726532	7.893671413	7.291768677			
Ce	5.796757803	1.089298875	7.179400478			
Ce	4.075159776	4.416919088	7.098955051			
Ce	1.971661392	7.996775142	7.131758070			
Ce	9.734978295	1.090238835	7.179720992			
Ce	7.835776041	4.543952186	7.197406468			
Ce	5.922881366	7.896286385	7.280745372			
Ce	0.005374637	2.221805890	3.932465586			
Ce	-1.907514436	5.639261554	3.987426349			
Ce	-3.878970781	8.968872472	3.967833923			
Ce	3.880668111	2.240656476	3.958993696			
Ce	1.953949097	5.610442068	4.023936234			
Ce	-0.003927412	8.971727596	3.967447849			
Ce	7.792907867	2.242658499	4.015917398			
Ce	5.852546662	5.645271910	3.969185162			
Ce	3.907805695	8.964823220	3.966279590			
Pt	2.198493069	5.816374429	11.157104543			
Pt	2.086671490	4.194219964	9.281571828			
Pt	3.576016742	6.477502461	9.146485195			
Pt	0.638136980	6.452482776	9.263544609			

Pt₄/ CeO₂(111) – “Iso3_2D” (+0.60 eV)

85

O	-0.016168258	0.018061988	3.171073544			
O	-1.961357033	3.377321118	3.168603367			
O	-3.876054926	6.752612180	3.142915526			
O	3.900217111	-0.011769054	3.137007748			
O	1.931364882	3.362263563	3.155449526			
O	0.005915497	6.751552433	3.156214170			
O	7.782851362	0.017191862	3.165956353			
O	5.851447373	3.328242070	3.172560613			
O	3.905636402	6.764924058	3.151969195			
O	0.050802594	2.267813078	6.280500552			
O	-1.958002033	5.636240149	6.310434087			
O	-3.862936038	9.004703434	6.335206586			
O	3.887605926	2.279940699	6.337311152			
O	2.006165540	5.600558691	6.310275206			
O	0.071312540	8.820472839	6.510410203			
O	7.574807289	2.339380228	6.416826459			
O	5.737528567	5.626051686	6.435778890			
O	3.978084805	9.033917576	6.270477956			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	0.061659980	0.083379858	7.911897876			
O	-1.878611545	3.316546916	7.854501028			
O	-3.901938320	6.841733968	7.969542856			
O	3.902065196	-0.027338218	7.940064030			
O	1.449189819	2.980040852	8.356398566			
O	-0.768563856	6.384079772	8.493860083			
O	7.873686501	0.066621372	7.911339466			
O	7.295335880	3.750817599	9.206167524			
O	4.190906382	7.806702824	8.617373818			
O	1.970877257	1.106614055	4.757580500			
O	-0.007527409	4.525978963	4.774046712			
O	-1.925110528	7.890166408	4.792776478			
O	5.803133176	1.011779446	4.831592101			
O	3.911506532	4.484621799	4.613418420			

O	1.983097114	7.892766866	4.773570189			
O	9.673339506	1.191852642	4.833911400			
O	7.755478994	4.537641043	4.780760204			
O	5.884873865	7.852212281	4.772492213			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.944881561	1.056883249	7.122108078			
Ce	-0.104878027	4.491261696	7.170575815			
Ce	-1.985230112	7.842027663	7.222125393			
Ce	5.835707456	0.954945088	7.159297159			
Ce	3.882115836	4.474682394	6.849304151			
Ce	2.163348215	8.042096862	7.173003688			
Ce	9.767446674	1.185318404	7.140148017			
Ce	7.842894658	4.571504376	7.266695615			
Ce	5.942941392	7.979563615	7.195162655			
Ce	-0.006366785	2.275063200	3.958772715			
Ce	-1.954746421	5.620184436	3.968409710			
Ce	-3.879277896	8.984746443	3.952444584			
Ce	3.886681129	2.197644922	3.922921885			
Ce	1.927822683	5.640244651	3.940393184			
Ce	0.015388205	8.954792828	3.974789297			
Ce	7.755520349	2.270051770	4.005730480			
Ce	5.874212512	5.648652260	3.947601819			
Ce	3.901812790	9.004287426	3.936335780			
Pt	5.426227969	3.319338023	9.062966688			
Pt	2.972260763	3.570964816	9.418455913			
Pt	3.676383420	5.990681269	9.205266883			

Pt₅/ CeO₂(111) – GM (0.0 eV)

86

O	-0.031685359	0.002268710	3.176858315			
O	-1.934859073	3.353866313	3.146785991			
O	-3.880685102	6.748758742	3.148843453			
O	3.899314220	-0.009119966	3.167592982			
O	1.920592950	3.390922846	3.136191839			
O	0.016227313	6.741855356	3.153631119			
O	7.792113616	-0.031702157	3.161842847			
O	5.858329713	3.363531745	3.159257857			
O	3.875426492	6.777887136	3.173126261			
O	-0.053052937	2.191212354	6.307180893			
O	-1.917033563	5.604628383	6.441890028			
O	-3.783625269	9.140427575	6.272210822			
O	3.908079895	2.267474220	6.273240009			
O	1.985538515	5.536474554	6.414262534			
O	-0.097132644	9.012529435	6.444242120			
O	7.698330787	2.312106887	6.421854665			
O	5.855801731	5.498942693	6.226727762			
O	3.932859047	8.969483160	6.377673311			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.001410409	-0.068565531	8.169150367			
O	-1.948232768	3.282949018	7.959987626			
O	-3.862724820	6.769741053	7.781685672			
O	3.730601282	-1.312653594	9.393203644			
O	1.193096175	3.255426652	8.489957723			
O	0.095645379	6.746034186	7.978050324			
O	7.845791779	-0.048420265	7.910645117			
O	7.002553842	4.323034295	9.393866362			
O	3.959038791	6.790804669	8.103752988			
O	1.920648761	1.194435704	4.716320646			
O	-0.005946680	4.502033923	4.805114118			
O	-1.917134216	7.820231908	4.784309587			
O	5.877112709	1.088072534	4.736329871			
O	3.870198329	4.510950029	4.656397314			

O	1.905172492	7.853462483	4.878963449			
O	9.658165408	1.123297203	4.838096286			
O	7.857477997	4.489611337	4.755407830			
O	5.872677908	7.862439141	4.804424243			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.820953760	1.233068081	7.061604972			
Ce	-0.088950861	4.509137359	7.224456735			
Ce	-1.941917841	7.808664434	7.253163951			
Ce	5.974632152	1.043055689	7.047229341			
Ce	3.923570697	4.567350936	6.935294041			
Ce	1.940331903	7.835186399	7.205116370			
Ce	9.704835342	1.122940621	7.186465253			
Ce	7.858946311	4.530979467	7.278900390			
Ce	5.886406786	7.859789443	7.114440480			
Ce	-0.021715726	2.256298631	3.937446948			
Ce	-1.944607065	5.614819100	3.981209235			
Ce	-3.871691723	8.999096295	3.969074856			
Ce	3.888630580	2.243212047	3.936448676			
Ce	1.918921384	5.615682587	3.948750045			
Ce	-0.012298341	8.963204722	3.962585621			
Ce	7.793231517	2.263558396	3.957273712			
Ce	5.882978839	5.617876357	3.925304307			
Ce	3.884493907	8.986912113	3.983485810			
Pt	4.007603330	0.691855984	9.143323728			
Pt	1.775231804	-0.711174525	9.103183576			
Pt	5.358948646	5.547842031	9.080939824			
Pt	5.638594612	2.778191752	9.232080707			
Pt	3.082207198	3.068732427	9.133087992			

Pt₅/ CeO₂(111) – GM (0.0 eV)

86

O	-0.031685359	0.002268710	3.176858315			
O	-1.934859073	3.353866313	3.146785991			
O	-3.880685102	6.748758742	3.148843453			
O	3.899314220	-0.009119966	3.167592982			
O	1.920592950	3.390922846	3.136191839			
O	0.016227313	6.741855356	3.153631119			
O	7.792113616	-0.031702157	3.161842847			
O	5.858329713	3.363531745	3.159257857			
O	3.875426492	6.777887136	3.173126261			
O	-0.053052937	2.191212354	6.307180893			
O	-1.917033563	5.604628383	6.441890028			
O	-3.783625269	9.140427575	6.272210822			
O	3.908079895	2.267474220	6.273240009			
O	1.985538515	5.536474554	6.414262534			
O	-0.097132644	9.012529435	6.444242120			
O	7.698330787	2.312106887	6.421854665			
O	5.855801731	5.498942693	6.226727762			
O	3.932859047	8.969483160	6.377673311			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.001410409	-0.068565531	8.169150367			
O	-1.948232768	3.282949018	7.959987626			
O	-3.862724820	6.769741053	7.781685672			
O	3.730601282	-1.312653594	9.393203644			
O	1.193096175	3.255426652	8.489957723			
O	0.095645379	6.746034186	7.978050324			
O	7.845791779	-0.048420265	7.910645117			
O	7.002553842	4.323034295	9.393866362			
O	3.959038791	6.790804669	8.103752988			
O	1.920648761	1.194435704	4.716320646			
O	-0.005946680	4.502033923	4.805114118			
O	-1.917134216	7.820231908	4.784309587			
O	5.877112709	1.088072534	4.736329871			
O	3.870198329	4.510950029	4.656397314			

O	1.905172492	7.853462483	4.878963449			
O	9.658165408	1.123297203	4.838096286			
O	7.857477997	4.489611337	4.755407830			
O	5.872677908	7.862439141	4.804424243			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.820953760	1.233068081	7.061604972			
Ce	-0.088950861	4.509137359	7.224456735			
Ce	-1.941917841	7.808664434	7.253163951			
Ce	5.974632152	1.043055689	7.047229341			
Ce	3.923570697	4.567350936	6.935294041			
Ce	1.940331903	7.835186399	7.205116370			
Ce	9.704835342	1.122940621	7.186465253			
Ce	7.858946311	4.530979467	7.278900390			
Ce	5.886406786	7.859789443	7.114440480			
Ce	-0.021715726	2.256298631	3.937446948			
Ce	-1.944607065	5.614819100	3.981209235			
Ce	-3.871691723	8.999096295	3.969074856			
Ce	3.888630580	2.243212047	3.936448676			
Ce	1.918921384	5.615682587	3.948750045			
Ce	-0.012298341	8.963204722	3.962585621			
Ce	7.793231517	2.263558396	3.957273712			
Ce	5.882978839	5.617876357	3.925304307			
Ce	3.884493907	8.986912113	3.983485810			
Pt	4.007603330	0.691855984	9.143323728			
Pt	1.775231804	-0.711174525	9.103183576			
Pt	5.358948646	5.547842031	9.080939824			
Pt	5.638594612	2.778191752	9.232080707			
Pt	3.082207198	3.068732427	9.133087992			

Pt₅/ CeO₂(111) – “Iso1_2D” (+0.36 eV)

86

O	-0.026800266	-0.009322066	3.186058931			
O	-1.936385842	3.364346676	3.150454168			
O	-3.889819056	6.740088130	3.153595117			
O	3.900835448	-0.026941970	3.153091876			
O	1.906938310	3.386942252	3.130290945			
O	0.013862108	6.740835063	3.146595440			
O	7.803373911	-0.016072001	3.156863178			
O	5.863107036	3.364771713	3.151607719			
O	3.875390783	6.774433301	3.180860582			
O	0.013738026	2.171751089	6.288424683			
O	-1.956554931	5.614760017	6.488064298			
O	-3.795952682	9.093872001	6.277213850			
O	3.917944185	2.218625135	6.263410130			
O	2.003187311	5.643039220	6.327478673			
O	-0.131377835	9.026719138	6.449268121			
O	7.703369104	2.292352054	6.409883090			
O	5.769212753	5.466368193	6.329027653			
O	3.953523399	8.998225852	6.370627613			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	0.029612063	-0.038475632	8.208257225			
O	-1.825098488	3.222752577	7.919404445			
O	-3.985541019	6.758447745	7.878143224			
O	3.762650091	-1.337897997	9.377919918			
O	1.589352707	3.413760870	8.114246585			
O	0.087772040	6.734696785	7.967564646			
O	7.828066588	-0.048537148	7.923932356			
O	7.418580588	3.916859038	9.326785629			
O	3.933304995	7.057536609	8.275789688			
O	1.950097889	1.160665355	4.693542056			
O	-0.021476304	4.515811762	4.814501231			
O	-1.918067004	7.800728511	4.789382383			
O	5.874433228	1.088639196	4.717828878			
O	3.860854668	4.473504120	4.610739230			

O	1.893078073	7.905493400	4.865555129			
O	9.681441893	1.152893088	4.837985202			
O	7.828570540	4.506029007	4.773303131			
O	5.873388958	7.818194144	4.833551357			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.865476586	1.212573148	7.031644232			
Ce	-0.056599500	4.536169546	7.168946297			
Ce	-1.969803097	7.789536571	7.286213224			
Ce	5.979078354	1.031088334	7.036900581			
Ce	3.809927723	4.464348520	6.847719334			
Ce	1.938058737	7.882866365	7.227275363			
Ce	9.744554401	1.129783209	7.191608300			
Ce	7.831940532	4.506386109	7.302136650			
Ce	5.859944847	7.848813586	7.167731017			
Ce	-0.014599517	2.247846267	3.936743016			
Ce	-1.960294247	5.617778013	3.990556099			
Ce	-3.878641566	8.974117350	3.975668227			
Ce	3.894574351	2.214243733	3.900584566			
Ce	1.915025769	5.645754604	3.924671190			
Ce	-0.006312392	8.963859160	3.962951924			
Ce	7.799922485	2.261005119	3.959353250			
Ce	5.876496798	5.614101946	3.955821162			
Ce	3.886981019	8.994391475	3.994175595			
Pt	4.129922591	0.680293261	9.193678594			
Pt	1.833736169	-0.648519229	9.093666974			
Pt	4.606424922	5.326192988	9.189064204			
Pt	5.810202833	2.790554497	9.285473330			
Pt	3.280237540	3.031922785	9.225586838			

Pt₅ / CeO₂(111) – “Iso2_2D” (+0.51 eV)

86

O	-0.004488103	-0.036468378	3.184233208			
O	-1.944549197	3.381027535	3.157695630			
O	-3.888611259	6.736991111	3.145634842			
O	3.912177384	-0.025568301	3.143889536			
O	1.915846867	3.384712646	3.143561070			
O	-0.013271371	6.743352887	3.164555921			
O	7.797386042	-0.014065302	3.131088855			
O	5.873531147	3.374608610	3.134957753			
O	3.881737122	6.775223110	3.191001445			
O	-0.017903484	2.000378106	6.290567105			
O	-2.043827734	5.663531362	6.392051819			
O	-3.895212710	9.054894057	6.447975198			
O	4.036753204	2.199403541	6.234136351			
O	2.083210813	5.755172542	6.255092871			
O	-0.152959717	9.118609533	6.465221071			
O	7.814530546	2.269521353	6.272973826			
O	5.766607843	5.516604405	6.446813543			
O	3.940827846	8.939158443	6.335582050			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.567318194	-0.298498500	8.470741621			
O	-1.980949938	3.308903466	7.964732812			
O	-3.991133280	6.703356809	8.023469527			
O	4.103722858	-1.224722748	9.184869239			
O	1.868198176	3.401827534	7.570705947			
O	0.053788230	6.802304897	7.939122766			
O	7.821496449	0.002514757	7.920910189			
O	6.768096125	2.973269856	8.573756374			
O	3.803862687	7.187626456	8.391040745			
O	1.995952209	1.119874662	4.606982773			
O	-0.024017989	4.491082406	4.794351065			
O	-1.970180659	7.858868972	4.792417411			
O	5.910895047	1.107541568	4.716979872			
O	3.897338866	4.471865198	4.586328562			

O	1.860974316	7.953857444	4.825337236			
O	9.699317668	1.102957918	4.762172102			
O	7.775145354	4.527700386	4.794158995			
O	5.903429893	7.799007917	4.859268951			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	2.012274904	1.166670282	6.823919016			
Ce	-0.108142079	4.552276873	7.184671937			
Ce	-1.975334678	7.781055561	7.300979752			
Ce	6.066483846	1.129181786	7.090738565			
Ce	3.815130131	4.459750129	6.799844397			
Ce	1.890749238	7.906733788	7.195751658			
Ce	9.723343367	1.109488299	7.187933245			
Ce	7.859749519	4.487681913	7.216234790			
Ce	5.824905327	7.818069379	7.267678620			
Ce	-0.031563020	2.243563663	3.934309031			
Ce	-1.955671592	5.626730653	3.982346694			
Ce	-3.887926745	8.934395499	3.961230505			
Ce	3.953295951	2.220524351	3.860502646			
Ce	1.899714924	5.650163999	3.925353305			
Ce	-0.015738430	8.994994064	3.976387662			
Ce	7.812123483	2.239349699	3.927413745			
Ce	5.876999099	5.631039449	3.953241057			
Ce	3.883239392	8.988730690	3.986364283			
Pt	3.841328346	0.677058998	9.216182138			
Pt	1.044717990	0.605058143	9.206988558			
Pt	3.753841097	5.362744746	9.256492216			
Pt	4.917776049	3.031786634	9.220725482			
Pt	2.395863007	2.885897463	9.407029035			

Pt₅/ CeO₂(111) – “Iso3_3D” (+1.01 eV)

86

O	-0.027926341	-0.003431417	3.174691619			
O	-1.932722521	3.351919518	3.136048100			
O	-3.886011139	6.750784725	3.136291913			
O	3.895477764	-0.017231293	3.155204378			
O	1.921061600	3.386604178	3.128905847			
O	0.018001012	6.746979460	3.142465905			
O	7.803100488	-0.031263250	3.164774012			
O	5.864354116	3.373766809	3.146513162			
O	3.885863461	6.781923885	3.169853075			
O	0.016334377	2.214791792	6.305558811			
O	-1.898335369	5.591710217	6.471332450			
O	-3.786033519	9.155497026	6.391511661			
O	3.893608992	2.275863805	6.314795003			
O	2.009511921	5.506024650	6.404632594			
O	-0.099674346	9.048608482	6.431086275			
O	7.667207356	2.311910126	6.411758858			
O	5.840105548	5.503828754	6.231562643			
O	3.931040084	8.941430749	6.363148919			
O	1.945943512	1.123508622	-0.007458684	0	0	0
O	-0.000065583	4.493950135	-0.007364606	0	0	0
O	-1.945992233	7.864467697	-0.007363162	0	0	0
O	5.837819924	1.123473163	-0.007269874	0	0	0
O	3.891879044	4.493954315	-0.007202975	0	0	0
O	1.945973422	7.864495846	-0.007283114	0	0	0
O	9.729789468	1.123537315	-0.007272123	0	0	0
O	7.783893843	4.493966618	-0.007215649	0	0	0
O	5.837915971	7.864501561	-0.007173318	0	0	0
O	-0.000002077	2.246992724	1.603764045	0	0	0
O	-1.945928584	5.617430747	1.603765689	0	0	0
O	-3.891883464	8.988005991	1.603833932	0	0	0
O	3.891885581	2.246981810	1.603838953	0	0	0
O	1.945922669	5.617450509	1.603766532	0	0	0
O	-0.000016518	8.987997589	1.603801497	0	0	0
O	7.783841637	2.247030278	1.603822149	0	0	0
O	5.837892778	5.617459095	1.603804665	0	0	0
O	3.891925509	8.988016142	1.603780083	0	0	0
O	-0.011049320	-0.004719207	8.048137835			
O	-1.943339451	3.250191610	7.952199494			
O	-3.867532085	6.806036914	7.778041930			
O	3.757595790	-1.339447786	9.271177531			
O	1.198958583	3.298865084	8.458137982			
O	0.154414375	6.770461581	7.973196925			
O	7.844783714	-0.041498501	7.919686043			
O	7.048258897	4.306388352	9.412040462			
O	3.932983660	6.785085533	8.154161509			
O	1.935202852	1.164585134	4.723885793			
O	-0.007437492	4.508708362	4.797135297			
O	-1.939397455	7.819434142	4.789124557			
O	5.862818173	1.102380109	4.726601261			
O	3.879193718	4.502535980	4.659440653			

O	1.898068665	7.841985308	4.888821150			
O	9.677443547	1.141118305	4.858726698			
O	7.867719462	4.500376960	4.766047921			
O	5.901029238	7.867701717	4.829020367			
Ce	0.000034891	0.000035348	0.790754446	0	0	0
Ce	-1.945940043	3.370523402	0.790768980	0	0	0
Ce	-3.891876564	6.741033272	0.790804396	0	0	0
Ce	3.891878580	0.000053748	0.790779682	0	0	0
Ce	1.945934797	3.370452531	0.790735408	0	0	0
Ce	-0.000011749	6.740956919	0.790739214	0	0	0
Ce	7.783804261	0.000034103	0.790779091	0	0	0
Ce	5.837875435	3.370504547	0.790810310	0	0	0
Ce	3.891908164	6.740915165	0.790819701	0	0	0
Ce	1.758967161	1.153494971	7.125223921			
Ce	-0.086285203	4.513970867	7.198685029			
Ce	-1.945623304	7.816054947	7.315292270			
Ce	5.972442659	1.049933029	7.065857957			
Ce	3.929938281	4.574032832	6.944711481			
Ce	1.925010788	7.840618605	7.229206888			
Ce	9.718525241	1.111030574	7.215162001			
Ce	7.863989790	4.530306906	7.290424348			
Ce	5.889883574	7.893116932	7.188339706			
Ce	-0.012244124	2.251186643	3.940423492			
Ce	-1.948716590	5.618528150	3.992270572			
Ce	-3.870251866	8.992992768	3.982187400			
Ce	3.888266043	2.239657575	3.948019443			
Ce	1.924972320	5.617400298	3.947376020			
Ce	-0.012980672	8.966498805	3.971657814			
Ce	7.796258164	2.263981731	3.964793673			
Ce	5.884890765	5.622762478	3.934971669			
Ce	3.889231892	8.984794524	4.002876808			
Pt	3.992666378	0.565979807	9.222206662			
Pt	4.218858680	2.170726898	11.139115745			
Pt	5.372945564	5.535484981	9.094927557			
Pt	5.636157675	2.840733372	9.201916759			
Pt	2.968342041	3.019202001	9.236152839			

Pt₆/ CeO₂(111) – GM (0.0 eV)

150

O	0.020458345	-0.005487865	3.172155236			
O	-1.960513618	3.351011052	3.142386007			
O	-3.905296851	6.742399993	3.165383074			
O	-5.824479550	10.113585265	3.159464328			
O	3.894960172	-0.009526065	3.161133628			
O	1.922752976	3.362971310	3.156816841			
O	-0.017700388	6.744743438	3.142608758			
O	-1.960532763	10.119050376	3.166697431			
O	7.773200978	0.002314499	3.166931629			
O	5.870001133	3.340586189	3.143807995			
O	3.850651797	6.771211469	3.122239751			
O	1.940267833	10.120988156	3.154930422			
O	11.685952108	0.035046659	3.132918097			
O	9.755102224	3.341428911	3.148181067			
O	7.831527198	6.726717142	3.141282045			
O	5.842190547	10.143350777	3.164188508			
O	0.010107667	2.270394044	6.317198429			
O	-1.992032498	5.596273189	6.358558762			
O	-3.889081459	8.989682225	6.362421594			
O	-5.800672032	12.380847741	6.369492187			
O	3.894535657	2.389412709	6.431863041			
O	1.750265380	5.404185547	6.333225779			
O	-0.068324650	8.986536877	6.331687971			
O	-1.952604244	12.348527382	6.367720681			
O	7.821723887	2.209905201	6.326714114			
O	6.054615457	5.510542744	6.265759004			
O	4.102519247	9.374971885	6.257237783			
O	1.966175373	12.316241194	6.418723259			
O	11.697076744	2.218260538	6.331059903			
O	9.773047224	5.598512035	6.334483922			
O	7.687137898	8.909741353	6.461539345			
O	5.863019640	12.354869457	6.338533764			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	0.042585929	0.041432128	7.910628141			
O	-2.000655192	3.341567020	7.968424199			
O	-3.861737448	6.766297378	7.971286986			
O	-5.790643545	10.126189118	7.968408258			
O	3.911810458	0.014570583	7.958271064			
O	1.356074889	3.068765805	8.483484054			
O	-0.079892733	6.742445701	7.940995637			
O	-1.987587105	10.126304943	7.990356317			
O	7.783379196	-0.044314097	7.961847322			
O	6.449253209	2.951064253	8.440399174			
O	3.766529239	6.859000038	6.245283435			
O	1.618383581	10.031243636	8.191734383			
O	11.702655863	0.036724515	7.968376958			
O	9.819578413	3.298750002	7.954773903			
O	8.440369064	6.409533791	8.451597371			
O	6.114691437	10.818532901	8.554789083			
O	1.984702360	1.128460267	4.808404932			
O	-0.078261841	4.488808137	4.728687142			
O	-1.973596061	7.851570517	4.788103536			
O	-3.890841370	11.233019367	4.802330592			
O	5.808795939	1.118062263	4.825206114			
O	3.908010966	4.479637123	4.556390936			
O	1.844510221	7.907628197	4.757987891			
O	-0.006689877	11.250397698	4.801428224			
O	9.742337976	1.085353359	4.805637457			
O	7.864628833	4.443282245	4.735199657			
O	5.882513480	7.861578418	4.556892309			
O	3.875463929	11.366657353	4.707381744			
O	13.642596800	1.116035203	4.793418386			
O	11.682813290	4.472261421	4.782548747			
O	9.719664254	7.887347837	4.828871561			
O	7.830872664	11.209664712	4.819104133			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.130281145	4.455463482	7.189002388			
Ce	-1.987539612	7.869181632	7.157174092			
Ce	-3.877290946	11.240501524	7.171793191			
Ce	5.869915740	1.061799113	7.207648656			
Ce	3.913538200	4.681875725	6.786420887			
Ce	1.757379035	7.774065120	7.074534494			
Ce	-0.059093286	11.231645875	7.184652250			
Ce	9.737608478	1.089264024	7.139270564			
Ce	7.959773203	4.386523715	7.205671755			
Ce	5.680744774	7.798644869	6.795552203			
Ce	3.952140577	11.402899960	7.150883846			
Ce	13.655514217	1.132476020	7.127856167			
Ce	11.686029420	4.473655902	7.131179265			
Ce	9.803763525	7.864768449	7.205165599			
Ce	7.884756577	11.288460093	7.194434238			
Ce	-0.001770953	2.261188895	3.952572356			
Ce	-1.959075516	5.604666547	3.955482286			
Ce	-3.898152149	8.981353878	3.974446106			
Ce	-5.828538059	12.357291923	3.972894469			
Ce	3.899735155	2.216998309	3.952889035			
Ce	1.904778630	5.639764727	3.917146697			
Ce	-0.038788037	9.007172902	3.952591469			
Ce	-1.943919261	12.362343052	3.975828192			
Ce	7.802270302	2.237283990	3.962322294			
Ce	5.901364051	5.591135277	3.877829934			
Ce	3.864761600	9.018999085	3.930347469			
Ce	1.946646170	12.364753202	3.962532197			
Ce	11.684941724	2.233317076	3.952368926			
Ce	9.743106770	5.596569858	3.960905496			
Ce	7.821416162	9.006007092	3.963059697			
Ce	5.845375844	12.365494338	3.950738897			
Pt	6.613123689	6.699682949	9.229095687			
Pt	5.377250652	4.454941437	9.245693375			
Pt	2.815239295	4.195225572	9.225137018			
Pt	3.898341283	6.632261918	9.305798562			
Pt	3.135051288	9.188439106	9.212091434			
Pt	5.648475755	9.065263520	9.305460816			

Pt₆/ CeO₂(111) – “Iso1_2D” (+0.68 eV)

150

O	0.015109201	-0.006993473	3.178364572			
O	-1.965540794	3.366235648	3.162466291			
O	-3.884222496	6.744304054	3.155163671			
O	-5.831539053	10.122055443	3.166756163			
O	3.893135650	-0.005603474	3.165595448			
O	1.932265903	3.362957464	3.152776545			
O	-0.017150326	6.758266692	3.152133765			
O	-1.948172632	10.117714293	3.173295067			
O	7.788720264	-0.000568493	3.155969716			
O	5.834749366	3.348094310	3.145114676			
O	3.855425351	6.767709759	3.123563929			
O	1.927600779	10.126843965	3.151874061			
O	11.670268624	0.026877457	3.163570615			
O	9.750522444	3.361180000	3.164037345			
O	7.805499724	6.763039386	3.147010329			
O	5.843228335	10.136345336	3.158305975			
O	0.011755769	2.264105652	6.331567867			
O	-1.911032981	5.583657630	6.350717621			
O	-3.868141306	9.017716987	6.386554641			
O	-5.872093476	12.390897658	6.329993266			
O	3.941528659	2.358916307	6.387823879			
O	1.849147268	5.529087829	6.286707278			
O	-0.044723840	9.026167472	6.331528723			
O	-1.940102615	12.340895229	6.381943705			
O	7.777536482	2.331209620	6.423857749			
O	5.843251326	5.618956982	6.223263604			
O	3.938102239	9.147336969	6.283870101			
O	1.990202488	12.372717576	6.362532311			
O	11.717808455	2.229415764	6.317534456			
O	9.677039228	5.604980810	6.396469605			
O	7.720120504	8.903090117	6.413219900			
O	5.839078767	12.355764475	6.349483621			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	-0.004091867	0.020906312	7.950581354			
O	-1.915657180	3.366468501	7.979625510			
O	-3.736101865	6.734253829	7.947384971			
O	-5.812800832	10.226141531	7.963749365			
O	3.823799953	-0.068335235	7.934483180			
O	1.653313473	3.181866765	8.259072148			
O	-0.039703098	6.777007239	7.972684113			
O	-1.931437953	10.123301391	8.004372119			
O	7.863752428	-0.080085616	7.966909623			
O	5.789677995	2.072752730	9.136835199			
O	3.612183926	6.942913136	7.808807276			
O	1.898702145	10.152511155	7.974335225			
O	11.693368554	0.003863146	7.986300930			
O	10.324054722	3.069231833	8.355418427			
O	9.068265402	7.196332937	9.120115955			
O	5.839547699	10.515792733	8.320847448			
O	1.984951872	1.146292976	4.803847891			
O	-0.038863577	4.486959423	4.747106296			
O	-1.957311987	7.859783873	4.796679534			
O	-3.892093730	11.243273655	4.802182127			
O	5.851604783	1.107380625	4.784893742			
O	3.873517994	4.529920615	4.628374695			
O	1.925332661	7.889249651	4.789523779			
O	0.007346153	11.257608302	4.797095844			
O	9.700526597	1.131235787	4.827259067			
O	7.790377365	4.496236454	4.618367049			
O	5.806735749	7.872739023	4.628527668			
O	3.882129469	11.293972074	4.751262190			
O	13.643605409	1.114812081	4.792302486			
O	11.668234883	4.521727942	4.818881080			
O	9.757143723	7.877602729	4.783211168			
O	7.790464362	11.202190709	4.824864389			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.052059604	4.487029411	7.185052102			
Ce	-1.933506503	7.877796370	7.184485246			
Ce	-3.893003464	11.247351070	7.171972240			
Ce	5.839696897	0.973331261	7.302596301			
Ce	3.801887022	4.595775886	6.862280838			
Ce	1.802133744	7.968139175	7.137416566			
Ce	-0.000350327	11.242920126	7.187179441			
Ce	9.785931553	1.071612065	7.211589780			
Ce	7.797877315	4.514119797	6.848431623			
Ce	5.715258769	7.900394162	6.859114883			
Ce	3.878745920	11.311788090	7.191795091			
Ce	13.645363348	1.122688781	7.139764215			
Ce	11.773950379	4.494153921	7.201342207			
Ce	9.875930809	7.950867483	7.306519602			
Ce	7.809150628	11.285731542	7.203680456			
Ce	0.001111191	2.254211154	3.963992670			
Ce	-1.953181802	5.609981907	3.972839845			
Ce	-3.892901309	8.991792392	3.984330549			
Ce	-5.839082062	12.361049066	3.981520137			
Ce	3.908663705	2.215774304	3.960583029			
Ce	1.881892108	5.633198547	3.914580455			
Ce	-0.023074770	9.008122886	3.957234046			
Ce	-1.943965235	12.366529283	3.982462606			
Ce	7.783560912	2.204122824	3.953188977			
Ce	5.828123549	5.629172168	3.844270535			
Ce	3.852337163	9.049248450	3.915323391			
Ce	1.952244382	12.379910107	3.975947867			
Ce	11.674234813	2.251879630	3.973086317			
Ce	9.773947409	5.649519648	3.948704233			
Ce	7.825939543	9.003663404	3.972294437			
Ce	5.840664304	12.360950006	3.971685082			
Pt	7.292679019	6.380947182	9.277607552			
Pt	6.155988738	3.985477933	9.326449255			
Pt	3.326140388	3.928358166	9.282972434			
Pt	4.787595472	6.129396168	9.307853240			
Pt	8.773834761	4.036645993	9.220405799			
Pt	5.947489902	8.671781302	9.288022348			

Pt₆/ CeO₂(111) – “Iso2_3D” (+1.91 eV)

150

O	0.003096629	-0.001549802	3.146231054			
O	-1.952656697	3.368577592	3.144091174			
O	-3.907459851	6.733705295	3.150693214			
O	-5.838872713	10.111132751	3.149792556			
O	3.912505940	0.020949546	3.152880642			
O	1.967288443	3.374546652	3.155941290			
O	-0.005062426	6.736074515	3.158350871			
O	-1.966026270	10.134655292	3.152964605			
O	7.754499980	0.029724885	3.162943401			
O	5.839616862	3.354535122	3.157178065			
O	3.898483633	6.749535197	3.155256655			
O	1.961519774	10.136078946	3.132827725			
O	11.685087986	-0.010118933	3.146119868			
O	9.739508080	3.394164277	3.149504432			
O	7.797800317	6.745701073	3.134498363			
O	5.849860075	10.127429427	3.135268994			
O	0.019782842	2.192098964	6.266951927			
O	-1.885681979	5.640424062	6.396525039			
O	-3.925621729	9.013182142	6.328135334			
O	-5.853815420	12.399276428	6.369005675			
O	3.793534590	2.396704334	6.454499649			
O	1.994628292	5.687370776	6.313209050			
O	-0.088095604	8.986082247	6.333394921			
O	-1.944072618	12.264608952	6.389869971			
O	7.836591020	2.306160813	6.325167637			
O	5.926107803	5.684079849	6.295674619			
O	3.950054358	8.816477837	6.361945854			
O	2.012934961	12.464632314	6.282509787			
O	11.658779723	2.251230963	6.339093333			
O	9.717715646	5.577580472	6.299525866			
O	7.799008601	9.015566165	6.333530893			
O	5.850312862	12.352049683	6.308018899			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	-0.066807087	-0.030180164	7.956744640			
O	-1.979440716	3.273404306	7.919797191			
O	-4.101565421	6.692044104	7.924952553			
O	-5.952543033	10.152240547	7.986746776			
O	3.928436610	0.073796171	7.954402502			
O	1.447686846	2.823867199	8.549918699			
O	-1.703468539	6.593673265	9.120481899			
O	-3.064613072	9.850013600	8.662461618			
O	7.811797372	0.125178280	7.905987708			
O	5.944175700	3.390156269	7.935020544			
O	4.889477297	6.505217765	8.393844966			
O	2.010989716	10.200246030	7.934965816			
O	11.739991077	-0.007328123	7.967088379			
O	9.782282079	3.404919964	8.000603646			
O	7.876716283	6.760887127	7.981131697			
O	5.864790330	10.164905671	7.974757967			
O	1.984817701	1.127943179	4.756664564			
O	0.003963282	4.462596078	4.741464927			
O	-1.984106328	7.858807815	4.734636492			
O	-3.918427301	11.263114610	4.772835837			
O	5.790375389	1.142857193	4.878529660			
O	3.951896434	4.523661820	4.762802744			
O	1.927817132	7.912051582	4.616738845			
O	0.025249467	11.266201293	4.720011212			
O	9.738086650	1.171506402	4.731377563			
O	7.780783041	4.509197198	4.758945906			
O	5.883350288	7.888518975	4.736118440			
O	3.919547027	11.191281117	4.794615628			
O	13.609814219	1.114508318	4.774417525			
O	11.709660360	4.506601513	4.811549123			
O	9.711954560	7.861044119	4.785676984			
O	7.797302384	11.244622454	4.778587903			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.119585501	4.284278509	7.095204140			
Ce	-2.197696247	7.891507152	7.387969873			
Ce	-3.993515277	11.261406006	7.240682135			
Ce	5.836142561	1.134098451	7.184991777			
Ce	4.164656393	4.556745884	7.102846605			
Ce	1.886517506	7.995455574	6.800585839			
Ce	0.118727226	11.402596734	7.106396495			
Ce	9.754788957	1.195189876	7.124832458			
Ce	7.867183871	4.516369931	7.147729947			
Ce	6.011957168	7.944199026	7.160742812			
Ce	3.978483553	11.275299051	7.145215229			
Ce	13.612704043	1.074909325	7.161875719			
Ce	11.675911608	4.498321977	7.160185686			
Ce	9.703416270	7.890475262	7.155469968			
Ce	7.787754699	11.265682963	7.178363637			
Ce	-0.004552976	2.233545824	3.926865396			
Ce	-1.946143987	5.647947291	3.987395355			
Ce	-3.894450718	8.984110443	3.983139216			
Ce	-5.823791815	12.357300639	3.969949643			
Ce	3.890239923	2.265458548	3.980798234			
Ce	1.952346317	5.597695748	3.962965150			
Ce	-0.080853988	9.002146744	3.943015505			
Ce	-1.974884202	12.366277815	3.986069243			
Ce	7.788345468	2.270065275	3.966161003			
Ce	5.868387940	5.643724914	3.941165499			
Ce	3.940739926	8.993184730	3.936120775			
Ce	1.958054233	12.373358095	3.928430823			
Ce	11.687620281	2.263402356	3.959537272			
Ce	9.736694501	5.623299516	3.957075860			
Ce	7.798768743	8.998711445	3.953604275			
Ce	5.854490134	12.359671837	3.947396437			
Pt	0.173695226	6.352964168	9.070806614			
Pt	1.318738610	8.740672976	9.305164539			
Pt	3.270308800	6.986330885	9.151508074			
Pt	1.712580005	6.478441634	11.007217709			
Pt	2.208156457	4.570850198	9.220917590			
Pt	-1.111706141	10.002328952	9.099379647			

Pt₇/CeO₂(111) – GM (0.0 eV)

151

O	0.023514933	-0.009537413	3.178627653			
O	-1.961296952	3.362702196	3.139686177			
O	-3.884957357	6.760943680	3.181155692			
O	-5.811194141	10.123796260	3.165132003			
O	3.901396576	-0.019109805	3.164853841			
O	1.926911203	3.351877966	3.141988293			
O	-0.031145654	6.738570497	3.144781820			
O	-1.955706095	10.123597597	3.165492362			
O	7.775387155	-0.011015127	3.182277070			
O	5.875918752	3.343574719	3.144884323			
O	3.900439372	6.745726329	3.094151104			
O	1.942685148	10.149338156	3.145884798			
O	11.681910959	0.022088092	3.141829220			
O	9.757709567	3.358654041	3.141625635			
O	7.831224549	6.732808868	3.147794225			
O	5.856748691	10.151169046	3.145060955			
O	-0.006227473	2.244738667	6.318236600			
O	-1.964975882	5.619636574	6.340405362			
O	-3.878242042	8.997616476	6.394240066			
O	-5.816846906	12.381086608	6.370922256			
O	3.905118610	2.382829274	6.448645296			
O	1.741077971	5.489373086	6.296053833			
O	0.115074614	8.924094993	6.472345274			
O	-1.929276283	12.354388991	6.384525274			
O	7.827411856	2.221318487	6.336269124			
O	6.088919542	5.495045990	6.297478522			
O	3.910454105	9.252971867	6.301594779			
O	1.952674627	12.388292487	6.339210133			
O	11.691997295	2.244491701	6.318018512			
O	9.779148972	5.614581909	6.338359464			
O	7.702053782	8.925909967	6.468232426			
O	5.862198275	12.391910388	6.335630016			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	0.036062080	0.014384404	7.942162904			
O	-2.010154153	3.329642789	7.964439755			
O	-3.875797162	6.773493589	7.978286768			
O	-5.803397317	10.147440626	7.979725435			
O	3.917102562	-0.001853420	7.959586259			
O	1.423733322	3.051575774	8.386323311			
O	-0.536051819	6.447717422	8.407407004			
O	-1.946412650	10.127245111	7.987681812			
O	7.780513617	-0.018207060	7.972611408			
O	6.408853428	3.018896405	8.405459131			
O	3.912410174	6.749759303	5.997943711			
O	1.945247325	10.726134262	8.388981158			
O	11.691662444	0.091761201	7.971256924			
O	9.832285258	3.325368636	7.969379818			
O	8.384568304	6.436662137	8.414734984			
O	5.885975081	10.747606509	8.403628346			
O	1.993517449	1.132874250	4.808515525			
O	-0.061470460	4.466907386	4.722452624			
O	-1.927271318	7.905336410	4.834850359			
O	-3.879785997	11.236256043	4.819998368			
O	5.814484520	1.115991427	4.832507428			
O	3.909543629	4.429497143	4.556585812			
O	1.893363335	7.904887037	4.565795726			
O	-0.012399170	11.204488862	4.834925638			
O	9.745910453	1.123627816	4.781696976			
O	7.870370466	4.452003334	4.731117092			
O	5.915429689	7.906944283	4.560173846			
O	3.904448828	11.315531050	4.730883177			
O	13.630940110	1.126689845	4.776962257			
O	11.687372434	4.491363159	4.784840034			
O	9.734832265	7.903638122	4.834042091			
O	7.823807352	11.208469676	4.833883667			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.141326113	4.419986023	7.217765669			
Ce	-1.988170874	7.880322273	7.220345754			
Ce	-3.878630178	11.250041541	7.181141087			
Ce	5.877822027	1.065398258	7.211838180			
Ce	3.918236015	4.635913073	6.779097563			
Ce	2.073991706	7.807511241	6.785680479			
Ce	-0.020114460	11.275624197	7.214541352			
Ce	9.749829395	1.120852854	7.131159134			
Ce	7.963316308	4.402416627	7.218586415			
Ce	5.749074464	7.808548573	6.781096164			
Ce	3.911529688	11.415742820	7.221110242			
Ce	13.637363702	1.129007303	7.124696273			
Ce	11.692660064	4.494121200	7.131703751			
Ce	9.805570712	7.879508547	7.215493771			
Ce	7.843175829	11.301320658	7.210211917			
Ce	-0.009359094	2.257824803	3.952054608			
Ce	-1.943909832	5.611481111	3.963553658			
Ce	-3.881426829	8.987243487	3.989757750			
Ce	-5.830146154	12.361253238	3.981922071			
Ce	3.909819602	2.198917385	3.941940198			
Ce	1.914876757	5.598383625	3.885080486			
Ce	-0.040811821	9.017394305	3.951439066			
Ce	-1.932808798	12.360634779	3.986995723			
Ce	7.809908931	2.246741359	3.963973189			
Ce	5.892344269	5.598967331	3.884780009			
Ce	3.902663407	9.037482750	3.886287348			
Ce	1.963568747	12.368252269	3.964492956			
Ce	11.683998721	2.246766718	3.949267821			
Ce	9.747215560	5.605613616	3.964649822			
Ce	7.846622562	9.019204064	3.951873838			
Ce	5.839668546	12.370703658	3.961687832			
Pt	6.597538196	6.764223477	9.254553800			
Pt	5.257826740	4.417984571	9.255485537			
Pt	2.640525838	4.395786677	9.245748264			
Pt	3.927098910	6.732243128	9.196690611			
Pt	2.586046145	9.038109265	9.261268620			
Pt	5.299621709	9.027071910	9.254369750			
Pt	1.257819272	6.774712891	9.249149805			

Pt₇/ CeO₂(111) – “Iso1_3D” (+1.18 eV)

151

O	-0.020808103	0.026342589	3.145971593			
O	-1.950274393	3.350953758	3.132570580			
O	-3.889989854	6.763422836	3.163053735			
O	-5.820029890	10.108552831	3.154101559			
O	3.902557796	-0.007459776	3.145722613			
O	1.919475511	3.358714228	3.145333042			
O	0.007426568	6.760093628	3.151486560			
O	-1.941299677	10.112882791	3.173701173			
O	7.780939637	-0.002184261	3.149251926			
O	5.846399014	3.330974875	3.119437640			
O	3.868943020	6.753805972	3.134270237			
O	1.943251000	10.110156905	3.161356740			
O	11.694231134	0.032367329	3.139739948			
O	9.766517936	3.354322947	3.148771239			
O	7.831321681	6.754686592	3.130473444			
O	5.846928741	10.146863659	3.168329004			
O	0.042407651	2.288744653	6.341578999			
O	-1.955475692	5.611000352	6.406657417			
O	-3.833077657	9.017265105	6.339889546			
O	-5.823168118	12.402248581	6.390775330			
O	3.799125458	2.224154926	6.299081670			
O	1.849378997	5.472068352	6.263807174			
O	-0.005509014	9.019463883	6.352457846			
O	-1.942708376	12.333220976	6.355113963			
O	7.870610126	2.217893717	6.302200008			
O	5.900069999	5.542636442	6.169690036			
O	4.012001271	9.161906956	6.249656146			
O	1.974295603	12.382443490	6.408281182			
O	11.631890816	2.295435418	6.388011142			
O	9.826143258	5.515418620	6.277823395			
O	7.673027396	9.152066772	6.323382246			
O	5.841757784	12.371382891	6.325070904			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	0.008910130	0.069507872	7.967451420			
O	-1.939880925	3.338824810	7.994780186			
O	-3.875726006	6.803090636	7.982700466			
O	-5.759464624	10.140658614	7.970310208			
O	3.923389902	-0.025044705	7.997182740			
O	1.643049837	3.206546840	8.328387221			
O	-0.005686739	6.780378245	7.958958391			
O	-1.948403638	10.116859191	8.022303142			
O	7.762623189	-0.008813520	8.005757949			
O	5.825311520	3.090861861	7.917471047			
O	3.780544204	6.764084405	7.354119214			
O	1.761895482	10.251079914	8.163187155			
O	11.701979370	0.050208155	7.987100130			
O	9.856223548	3.302359909	8.242537089			
O	8.000229369	6.837203227	7.592908736			
O	5.993715044	10.873566599	8.498378372			
O	1.930479428	1.097968894	4.760641641			
O	-0.074449545	4.495483355	4.750608593			
O	-1.927989826	7.856411262	4.813418764			
O	-3.899919044	11.250465033	4.806560493			
O	5.835262476	1.109782550	4.797619379			
O	3.895838122	4.468270227	4.622812539			
O	1.940918760	7.866667973	4.810147748			
O	0.018369869	11.256784619	4.803236203			
O	9.760386889	1.094967407	4.790583136			
O	7.824708158	4.462399544	4.630376443			
O	5.866228280	7.847040770	4.616460918			
O	3.872138424	11.329973795	4.751744398			
O	13.616326744	1.158292526	4.844010504			
O	11.741780923	4.490517550	4.766721871			
O	9.737405488	7.896895856	4.831333830			
O	7.831009367	11.305175382	4.761289917			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.036647879	4.482650311	7.183973685			
Ce	-1.945041568	7.889439615	7.184121848			
Ce	-3.880566096	11.251184823	7.196343467			
Ce	5.839994500	1.019686439	7.167385985			
Ce	3.931625524	4.436565350	6.857469380			
Ce	1.816696205	7.858189962	7.115363885			
Ce	-0.015884455	11.259408629	7.227049277			
Ce	9.746250620	1.108903347	7.199185183			
Ce	7.836649927	4.430247524	6.889886050			
Ce	5.857438835	7.809596974	6.831056449			
Ce	3.905311161	11.366833903	7.181232049			
Ce	13.640475860	1.165378661	7.180037651			
Ce	11.702072990	4.509195387	7.178518141			
Ce	9.852297188	7.950985184	7.141569971			
Ce	7.835474874	11.336745621	7.203556803			
Ce	-0.012552707	2.256134824	3.960511735			
Ce	-1.939394752	5.610813833	3.978371435			
Ce	-3.872981617	9.002981357	3.972841138			
Ce	-5.845167565	12.370352947	3.977045626			
Ce	3.878565442	2.195849982	3.917661676			
Ce	1.908077898	5.617110814	3.932070812			
Ce	0.001153473	9.006905480	3.975792937			
Ce	-1.937543131	12.352391668	3.977094292			
Ce	7.807411066	2.198073442	3.931933896			
Ce	5.858889343	5.596132720	3.841390839			
Ce	3.879706128	9.039635233	3.949722781			
Ce	1.962309554	12.373641707	3.984938784			
Ce	11.682252183	2.254268869	3.971636238			
Ce	9.782509654	5.623636868	3.939371488			
Ce	7.817968087	9.044603084	3.945176214			
Ce	5.842394168	12.388354787	3.967068624			
Pt	3.016564721	4.451634756	9.281539350			
Pt	5.350817582	5.923711814	11.313807750			
Pt	5.713618146	4.526156352	9.352634933			
Pt	7.084171540	6.779677458	9.396467658			
Pt	5.830640367	9.056924974	9.307888869			
Pt	4.302723270	6.839300278	9.329420820			
Pt	8.404947841	4.413928419	9.376755909			

Pt₇/ CeO₂(111) – “Iso2_2D” (+1.85 eV)

151

O	-0.013502403	0.025425185	3.145630365			
O	-1.949743839	3.361465658	3.140058460			
O	-3.886082654	6.763304904	3.168288057			
O	-5.817509849	10.118409373	3.158508062			
O	3.899918829	-0.013186721	3.157739384			
O	1.920656281	3.362044434	3.151461912			
O	-0.001306409	6.763629423	3.166598839			
O	-1.939303679	10.114589488	3.173882893			
O	7.784529910	-0.015680544	3.162768101			
O	5.843974643	3.322721386	3.133632333			
O	3.855563998	6.758355304	3.140561665			
O	1.933969405	10.114603603	3.171618139			
O	11.687952884	0.030759237	3.143922496			
O	9.760472802	3.351136068	3.156151476			
O	7.837408985	6.758631600	3.139498061			
O	5.846305324	10.150304389	3.166884073			
O	0.006993477	2.276359143	6.350890881			
O	-1.963638801	5.616671281	6.389063035			
O	-3.837892689	9.026027496	6.355348732			
O	-5.807565942	12.396886557	6.373941986			
O	3.794548740	2.223352766	6.282470978			
O	1.837802208	5.482944753	6.273153882			
O	-0.033405902	9.002205131	6.379939707			
O	-1.944921692	12.330332082	6.371044943			
O	7.888465208	2.222732984	6.298162594			
O	5.883184698	5.553322834	6.153834107			
O	4.085294542	9.211334224	6.238064374			
O	1.966699161	12.355369380	6.418085998			
O	11.649657425	2.281506225	6.381214742			
O	9.824008582	5.513895513	6.271405835			
O	7.650632351	9.169571120	6.304143427			
O	5.855982128	12.403406011	6.332741938			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	0.032021853	0.069156021	7.961845802			
O	-1.955518797	3.364953655	7.998056982			
O	-3.864500964	6.794432089	7.981903348			
O	-5.775256624	10.152033828	7.965201555			
O	3.910455097	-0.015504994	7.993310175			
O	1.675209936	3.223857507	8.264476949			
O	-0.046082120	6.738669483	7.980314550			
O	-1.960725972	10.124092110	8.030218642			
O	7.777423416	-0.012693494	7.997538809			
O	5.814914346	3.123585915	7.858446547			
O	3.780121287	6.756368194	7.354335371			
O	1.728726479	10.200580274	8.218815532			
O	11.703114344	0.057469618	7.982611692			
O	9.902313754	3.285882065	8.245177976			
O	7.979095756	6.845777910	7.554617115			
O	6.003352801	10.849009193	8.469256486			
O	1.917111264	1.107186085	4.763166419			
O	-0.067021059	4.489206068	4.757131908			
O	-1.940800878	7.867917580	4.809674374			
O	-3.886047305	11.243913956	4.802409417			
O	5.841906311	1.095659867	4.798636386			
O	3.885094194	4.473805555	4.608047109			
O	1.937389810	7.880613779	4.827730081			
O	0.005124637	11.241169464	4.820542737			
O	9.762059701	1.086407601	4.794907157			
O	7.817600453	4.466580386	4.615702396			
O	5.859134965	7.848555775	4.587815900			
O	3.881588737	11.340542898	4.745804998			
O	13.615465037	1.156964834	4.819180451			
O	11.732107769	4.485940863	4.766243622			
O	9.745244077	7.910459056	4.826597411			
O	7.822726415	11.314211968	4.757111171			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.062806205	4.473069905	7.175706460			
Ce	-1.959730372	7.877890588	7.188469869			
Ce	-3.878276063	11.256985939	7.195124875			
Ce	5.840039749	1.017012348	7.149410387			
Ce	3.907902031	4.440875896	6.837648931			
Ce	1.771868097	7.804508168	7.110553682			
Ce	-0.033607007	11.256835450	7.224541125			
Ce	9.750555369	1.103216082	7.191244964			
Ce	7.826558760	4.451675870	6.854466267			
Ce	5.853168512	7.821335391	6.807225937			
Ce	3.944690698	11.376423442	7.150529932			
Ce	13.635847648	1.161166255	7.159729056			
Ce	11.704691733	4.498540242	7.175797804			
Ce	9.860032441	7.959453967	7.127903481			
Ce	7.848239906	11.347409159	7.182372681			
Ce	-0.014401256	2.257466163	3.955917714			
Ce	-1.946350181	5.612717315	3.973449503			
Ce	-3.873673271	9.007858025	3.966763861			
Ce	-5.840851096	12.373904912	3.967448058			
Ce	3.875483550	2.196555753	3.915818496			
Ce	1.899983381	5.620055414	3.924640445			
Ce	-0.008153996	9.005917163	3.976247391			
Ce	-1.939001424	12.344938411	3.974355639			
Ce	7.809587157	2.193052583	3.931105881			
Ce	5.851767688	5.600400351	3.836779302			
Ce	3.883239548	9.046279162	3.937845927			
Ce	1.956873297	12.369895260	3.981663518			
Ce	11.683636893	2.251180272	3.965309123			
Ce	9.784009668	5.623991507	3.931044088			
Ce	7.813546384	9.050250734	3.938321255			
Ce	5.844902869	12.395817858	3.953386617			
Pt	3.037549047	4.429135170	9.277391993			
Pt	3.244782710	9.257099707	9.177073168			
Pt	5.733611794	4.529182132	9.324819760			
Pt	7.107765281	6.755649630	9.353084565			
Pt	5.848234438	9.034702998	9.312086306			
Pt	4.337414335	6.826605188	9.308890292			
Pt	8.427371900	4.395523846	9.332961232			

Pt₈/CeO₂(111) – GM (0.0 eV)

152

O	0.026570891	-0.014527994	3.178864801			
O	-1.963777206	3.357466613	3.132950722			
O	-3.899503337	6.761147743	3.174759976			
O	-5.806846936	10.122618947	3.172749196			
O	3.904067764	-0.028049188	3.172286484			
O	1.929394873	3.332775091	3.142907612			
O	-0.041724915	6.734278713	3.144716236			
O	-1.972625034	10.130432740	3.177708556			
O	7.766988853	0.001973440	3.175238700			
O	5.872986077	3.325467397	3.151970478			
O	3.909644786	6.737765845	3.084411716			
O	1.938591312	10.158146875	3.145794820			
O	11.684489293	0.027860573	3.135578193			
O	9.756523033	3.358860095	3.138373629			
O	7.843671108	6.742008034	3.154857865			
O	5.873321734	10.156492076	3.149115416			
O	0.010693335	2.227922209	6.314864225			
O	-1.961532654	5.598708683	6.331341455			
O	-3.838754105	9.044189269	6.493584027			
O	-5.797726689	12.364620761	6.419946943			
O	3.904712587	2.393380408	6.449000243			
O	1.725650461	5.501617874	6.287143664			
O	0.117521402	8.925270246	6.270872466			
O	-1.951109341	12.293503151	6.487151119			
O	7.815588668	2.233503795	6.338648074			
O	6.084651927	5.490254135	6.296000783			
O	3.893332996	9.257737284	6.289967917			
O	1.966375451	12.396340825	6.329989401			
O	11.685658554	2.250877574	6.293157397			
O	9.762677609	5.611994663	6.336255064			
O	7.686933745	8.916829473	6.474915369			
O	5.876276386	12.383429576	6.335172275			
O	1.945956000	1.123490000	0.001021000	0	0	0
O	-0.000006000	4.493961000	0.001121000	0	0	0
O	-1.946000000	7.864481000	0.000931000	0	0	0
O	-3.891953000	11.234965000	0.000876000	0	0	0
O	5.837850000	1.123506000	0.000808000	0	0	0
O	3.891925000	4.493984000	0.001009000	0	0	0
O	1.945969000	7.864460000	0.000941000	0	0	0
O	-0.000021000	11.234979000	0.000655000	0	0	0
O	9.729811000	1.123540000	0.000729000	0	0	0
O	7.783854000	4.494039000	0.000733000	0	0	0
O	5.837911000	7.864500000	0.000835000	0	0	0
O	3.891926000	11.234988000	0.000650000	0	0	0
O	13.621737000	1.123533000	0.000891000	0	0	0
O	11.675771000	4.494010000	0.000846000	0	0	0
O	9.729792000	7.864503000	0.000830000	0	0	0
O	7.783844000	11.234970000	0.000924000	0	0	0
O	0.000066000	2.247023000	1.598549000	0	0	0
O	-1.945920000	5.617441000	1.598583000	0	0	0

O	-3.891916000	8.987945000	1.598509000	0	0	0
O	-5.837929000	12.358604000	1.598550000	0	0	0
O	3.891780000	2.247055000	1.598517000	0	0	0
O	1.945983000	5.617420000	1.598591000	0	0	0
O	0.000013000	8.987938000	1.598556000	0	0	0
O	-1.946019000	12.358549000	1.598530000	0	0	0
O	7.783756000	2.246987000	1.598516000	0	0	0
O	5.837742000	5.617494000	1.598530000	0	0	0
O	3.891888000	8.987855000	1.598534000	0	0	0
O	1.945904000	12.358490000	1.598570000	0	0	0
O	11.675852000	2.247061000	1.598580000	0	0	0
O	9.729871000	5.617537000	1.598528000	0	0	0
O	7.783856000	8.987999000	1.598572000	0	0	0
O	5.837989000	12.358582000	1.598594000	0	0	0
O	0.031605689	0.014336298	7.949272502			
O	-2.021093252	3.290829412	7.948939963			
O	-3.883104896	6.730551050	7.969682729			
O	-5.833450215	10.134320780	8.045303165			
O	3.908130686	0.028152185	8.015983113			
O	1.440148451	3.032301567	8.414336006			
O	-0.585945827	6.209739656	8.474404029			
O	-1.812718564	10.043669473	8.243416219			
O	7.806334619	0.008676567	7.971538034			
O	6.464520786	3.034669226	8.467713928			
O	3.905302816	6.749493989	5.984074194			
O	2.124501858	10.904448756	8.468284905			
O	11.712588228	0.125259717	7.952904931			
O	9.837769472	3.320428254	7.955647396			
O	8.403031201	6.388441183	8.469622220			
O	5.901534746	10.769039510	8.457595019			
O	2.000332195	1.107816613	4.819348102			
O	-0.061375877	4.450125000	4.706186097			
O	-1.981087075	7.883405033	4.830592483			
O	-3.888481000	11.238140206	4.859448974			
O	5.808492956	1.080960711	4.876298908			
O	3.904468786	4.423276286	4.550943484			
O	1.917787975	7.888666062	4.528002606			
O	-0.023646277	11.262402084	4.828880075			
O	9.737291947	1.126743417	4.776233346			
O	7.866639199	4.451190995	4.717951836			
O	5.916159706	7.907263141	4.554765625			
O	3.913546536	11.323930580	4.711518103			
O	13.636835739	1.123014477	4.775730440			
O	11.682693255	4.496671904	4.776109579			
O	9.758567468	7.923486546	4.876268289			
O	7.842684879	11.210212429	4.854179873			
Ce	0.000031000	0.000040000	0.792349000	0	0	0
Ce	-1.945945000	3.370493000	0.792321000	0	0	0
Ce	-3.891919000	6.740983000	0.792328000	0	0	0
Ce	-5.837868000	10.111488000	0.792349000	0	0	0
Ce	3.891860000	0.000037000	0.792334000	0	0	0
Ce	1.945970000	3.370480000	0.792306000	0	0	0
Ce	0.000032000	6.740937000	0.792438000	0	0	0
Ce	-1.945962000	10.111477000	0.792329000	0	0	0

Ce	7.783813000	-0.000028000	0.792315000	0	0	0
Ce	5.837791000	3.370514000	0.792343000	0	0	0
Ce	3.891908000	6.740957000	0.792337000	0	0	0
Ce	1.945932000	10.111469000	0.792321000	0	0	0
Ce	11.675799000	0.000013000	0.792407000	0	0	0
Ce	9.729828000	3.370538000	0.792349000	0	0	0
Ce	7.783832000	6.741001000	0.792346000	0	0	0
Ce	5.837884000	10.111477000	0.792366000	0	0	0
Ce	1.945933000	1.123513000	7.151559000	0	0	0
Ce	-0.136533250	4.372713516	7.212003515			
Ce	-1.984288291	7.805243644	7.213886036			
Ce	-3.907673851	11.262806622	7.234478570			
Ce	5.893940915	1.075193342	7.241094424			
Ce	3.899800635	4.645989236	6.769901375			
Ce	2.057593960	7.813609569	6.748742339			
Ce	0.045624828	11.310219860	7.211547436			
Ce	9.761615407	1.131660842	7.122853472			
Ce	7.962497988	4.403382639	7.223783394			
Ce	5.729769655	7.809936948	6.772803317			
Ce	3.948961061	11.434940184	7.217473529			
Ce	13.636903499	1.127912825	7.123583642			
Ce	11.690905993	4.477611681	7.120667192			
Ce	9.803572891	7.862602545	7.243598138			
Ce	7.840821097	11.303213383	7.235529885			
Ce	-0.010052334	2.251602560	3.943265952			
Ce	-1.950247514	5.609158502	3.954781237			
Ce	-3.879427722	8.989852829	4.008552532			
Ce	-5.826087056	12.352640768	3.995580813			
Ce	3.910239458	2.188520976	3.947234600			
Ce	1.910483807	5.592859548	3.876407900			
Ce	-0.043085855	9.018585723	3.942720671			
Ce	-1.935830818	12.354029215	4.007393677			
Ce	7.809135486	2.244796478	3.960958649			
Ce	5.892520535	5.596094390	3.883162619			
Ce	3.903899058	9.041731140	3.878249562			
Ce	1.960297568	12.374497578	3.955837184			
Ce	11.683455085	2.246822734	3.939591176			
Ce	9.746818038	5.605673282	3.960518051			
Ce	7.851312881	9.022683750	3.961960546			
Ce	5.842604928	12.371850014	3.955026479			
Pt	6.586740313	6.831647003	9.220959416			
Pt	5.181541493	4.394275654	9.219615292			
Pt	2.568780257	4.457229530	9.256973466			
Pt	3.884200319	6.766741564	9.204092483			
Pt	2.517357198	9.080598446	9.228028047			
Pt	5.224626751	9.062587987	9.258636787			
Pt	1.193398317	6.782301111	9.228241741			
Pt	-0.155743655	9.089935107	9.147894959			

Pt₈/CeO₂(111) – “Iso1_3D” (+1.34 eV)

152

O	0.020220899	-0.005129793	3.181292268			
O	-1.958966634	3.367046745	3.144200046			
O	-3.882012246	6.761617910	3.180700128			
O	-5.813059616	10.123085148	3.165494881			
O	3.898088205	-0.019499041	3.165927929			
O	1.924848275	3.348497019	3.144679009			
O	-0.032541639	6.740358397	3.150650658			
O	-1.957590434	10.123432108	3.169326330			
O	7.776148224	-0.012137236	3.182612172			
O	5.876088944	3.342546957	3.149650568			
O	3.901224588	6.745429590	3.096304856			
O	1.945642836	10.150448507	3.150374636			
O	11.683843702	0.025007210	3.144872750			
O	9.759893536	3.357746998	3.144384822			
O	7.835861564	6.728161644	3.148773777			
O	5.856573021	10.152101189	3.152032880			
O	-0.012945268	2.247077763	6.321842091			
O	-1.962424669	5.619356286	6.338160495			
O	-3.877234866	9.002139815	6.395484899			
O	-5.823863737	12.382688097	6.369678930			
O	3.911087547	2.377550953	6.447918968			
O	1.746159084	5.501199923	6.309398844			
O	0.115307165	8.916484955	6.471136957			
O	-1.934895012	12.351234156	6.380850990			
O	7.832241902	2.213687321	6.331113433			
O	6.087906081	5.486048534	6.299027586			
O	3.926010079	9.249504433	6.298307656			
O	1.953924982	12.389304798	6.341127241			
O	11.692869860	2.252857954	6.317207027			
O	9.783752767	5.616113039	6.335431602			
O	7.709092279	8.923245082	6.461226933			
O	5.856674715	12.398014612	6.334008622			
O	1.945956000	1.123490000	0.001021000	0	0	0
O	-0.000006000	4.493961000	0.001121000	0	0	0
O	-1.946000000	7.864481000	0.000931000	0	0	0
O	-3.891953000	11.234965000	0.000876000	0	0	0
O	5.837850000	1.123506000	0.000808000	0	0	0
O	3.891925000	4.493984000	0.001009000	0	0	0
O	1.945969000	7.864460000	0.000941000	0	0	0
O	-0.000021000	11.234979000	0.000655000	0	0	0
O	9.729811000	1.123540000	0.000729000	0	0	0
O	7.783854000	4.494039000	0.000733000	0	0	0
O	5.837911000	7.864500000	0.000835000	0	0	0
O	3.891926000	11.234988000	0.000650000	0	0	0
O	13.621737000	1.123533000	0.000891000	0	0	0
O	11.675771000	4.494010000	0.000846000	0	0	0
O	9.729792000	7.864503000	0.000830000	0	0	0
O	7.783844000	11.234970000	0.000924000	0	0	0
O	0.000066000	2.247023000	1.598549000	0	0	0
O	-1.945920000	5.617441000	1.598583000	0	0	0

O	-3.891916000	8.987945000	1.598509000	0	0	0
O	-5.837929000	12.358604000	1.598550000	0	0	0
O	3.891780000	2.247055000	1.598517000	0	0	0
O	1.945983000	5.617420000	1.598591000	0	0	0
O	0.000013000	8.987938000	1.598556000	0	0	0
O	-1.946019000	12.358549000	1.598530000	0	0	0
O	7.783756000	2.246987000	1.598516000	0	0	0
O	5.837742000	5.617494000	1.598530000	0	0	0
O	3.891888000	8.987855000	1.598534000	0	0	0
O	1.945904000	12.358490000	1.598570000	0	0	0
O	11.675852000	2.247061000	1.598580000	0	0	0
O	9.729871000	5.617537000	1.598528000	0	0	0
O	7.783856000	8.987999000	1.598572000	0	0	0
O	5.837989000	12.358582000	1.598594000	0	0	0
O	0.030566022	0.017469648	7.946831342			
O	-2.012958447	3.335096810	7.971267484			
O	-3.866054734	6.772487125	7.975454462			
O	-5.803132789	10.152966133	7.979441527			
O	3.913670065	-0.010461773	7.960962651			
O	1.419636516	3.040259026	8.343945230			
O	-0.524762102	6.447926797	8.384527403			
O	-1.940168723	10.127480865	7.988240333			
O	7.777946140	-0.026836771	7.973699892			
O	6.431982960	3.008268323	8.391292596			
O	3.916875032	6.749990220	6.008207915			
O	1.948009766	10.680047327	8.353895434			
O	11.689915933	0.096336415	7.967224135			
O	9.834997947	3.322021483	7.966068321			
O	8.418214235	6.431652877	8.423284308			
O	5.889614241	10.745599174	8.391930568			
O	1.990325761	1.133507549	4.811832792			
O	-0.058130767	4.468915631	4.733868277			
O	-1.926737651	7.908365413	4.836320646			
O	-3.886345000	11.238350463	4.820012371			
O	5.814300081	1.109807630	4.830300830			
O	3.907265674	4.425892192	4.561235567			
O	1.898431723	7.911538774	4.574065315			
O	-0.013483191	11.202383277	4.838023654			
O	9.747954310	1.120605400	4.782910629			
O	7.871234736	4.449332224	4.733554372			
O	5.922612186	7.898488253	4.557008147			
O	3.901954185	11.318276952	4.733685115			
O	13.630186189	1.133188171	4.780430274			
O	11.689673124	4.496180432	4.783557588			
O	9.740518718	7.904907587	4.832808522			
O	7.821658041	11.211123901	4.833186172			
Ce	0.000031000	0.000040000	0.792349000	0	0	0
Ce	-1.945945000	3.370493000	0.792321000	0	0	0
Ce	-3.891919000	6.740983000	0.792328000	0	0	0
Ce	-5.837868000	10.111488000	0.792349000	0	0	0
Ce	3.891860000	0.000037000	0.792334000	0	0	0
Ce	1.945970000	3.370480000	0.792306000	0	0	0
Ce	0.000032000	6.740937000	0.792438000	0	0	0
Ce	-1.945962000	10.111477000	0.792329000	0	0	0

Ce	7.783813000	-0.000028000	0.792315000	0	0	0
Ce	5.837791000	3.370514000	0.792343000	0	0	0
Ce	3.891908000	6.740957000	0.792337000	0	0	0
Ce	1.945932000	10.111469000	0.792321000	0	0	0
Ce	11.675799000	0.000013000	0.792407000	0	0	0
Ce	9.729828000	3.370538000	0.792349000	0	0	0
Ce	7.783832000	6.741001000	0.792346000	0	0	0
Ce	5.837884000	10.111477000	0.792366000	0	0	0
Ce	1.945933000	1.123513000	7.151559000	0	0	0
Ce	-0.142723631	4.423696941	7.216431655			
Ce	-1.982809047	7.880870395	7.223001556			
Ce	-3.884892460	11.252104888	7.184006579			
Ce	5.879392829	1.057099987	7.214429240			
Ce	3.920591373	4.632784164	6.771849408			
Ce	2.078934734	7.817492810	6.790242204			
Ce	-0.023971298	11.270009377	7.217877503			
Ce	9.751176156	1.119986119	7.131311827			
Ce	7.972555298	4.401400067	7.221715005			
Ce	5.761997249	7.805513297	6.785683678			
Ce	3.913148560	11.412858012	7.221925675			
Ce	13.636367722	1.133057480	7.129894388			
Ce	11.696024305	4.498991118	7.134593417			
Ce	9.809785824	7.881334210	7.225021361			
Ce	7.838884412	11.304609033	7.216172725			
Ce	-0.008182206	2.262634544	3.961648682			
Ce	-1.940789117	5.613422352	3.970744365			
Ce	-3.880879258	8.987072722	3.997952868			
Ce	-5.834856065	12.362687953	3.989458722			
Ce	3.906540548	2.196262486	3.950026259			
Ce	1.914571120	5.602092928	3.894370914			
Ce	-0.038816740	9.016133174	3.960499556			
Ce	-1.934835041	12.359005296	3.992783467			
Ce	7.809989666	2.244094102	3.971446450			
Ce	5.893815854	5.593771199	3.887803911			
Ce	3.905283625	9.035130073	3.890978458			
Ce	1.964518397	12.367868495	3.972248191			
Ce	11.685909226	2.250267288	3.956484351			
Ce	9.749535820	5.606947085	3.971155761			
Ce	7.850460742	9.018782449	3.959322589			
Ce	5.839003177	12.374270370	3.969976165			
Pt	6.630635387	6.754518692	9.277965368			
Pt	5.306624421	4.375349299	9.276421155			
Pt	2.580586847	4.319512426	9.202332269			
Pt	3.982218784	6.732193860	9.189625294			
Pt	2.591416631	9.036902947	9.303069170			
Pt	5.316598837	9.027638819	9.275328350			
Pt	1.203182441	6.727090898	9.250819371			
Pt	3.735328663	4.951982008	11.088812247			

Pt₈/CeO₂(111) – “Iso2_3D” (+2.30 eV)

152

O	0.014715059	-0.006851481	3.178917161			
O	-1.965321012	3.366090599	3.163056681			
O	-3.883532136	6.744162950	3.155625385			
O	-5.831296256	10.122574493	3.167090493			
O	3.892793036	-0.005757478	3.166065811			
O	1.931813564	3.363010342	3.153520747			
O	-0.017218528	6.757959487	3.152966651			
O	-1.948044952	10.117656829	3.173938207			
O	7.789155069	-0.000999111	3.156407328			
O	5.834566653	3.348157399	3.145817523			
O	3.854903122	6.767679442	3.124351760			
O	1.927665059	10.127142196	3.152577012			
O	11.670595024	0.026757576	3.164144578			
O	9.751051097	3.360908546	3.164557080			
O	7.805528734	6.762811894	3.147495358			
O	5.842798690	10.137175479	3.158723215			
O	0.010677933	2.263841852	6.333085324			
O	-1.910706987	5.583277857	6.351223658			
O	-3.865289080	9.018979967	6.386015150			
O	-5.872364095	12.391360645	6.330070269			
O	3.940035126	2.360011535	6.388515606			
O	1.849572128	5.528771226	6.287988558			
O	-0.045324498	9.026610671	6.332079103			
O	-1.940105871	12.338698971	6.381903961			
O	7.779101302	2.332531399	6.424700080			
O	5.842207141	5.618101061	6.226717862			
O	3.937624112	9.146771885	6.284413025			
O	1.990524870	12.372502656	6.362820444			
O	11.719129400	2.229187572	6.318935044			
O	9.676444244	5.601963679	6.397037464			
O	7.719248206	8.904281419	6.413012264			
O	5.838875167	12.357397796	6.350218804			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	-0.005806240	0.022753672	7.952298298			
O	-1.915478157	3.364830278	7.981505319			
O	-3.733601820	6.732491022	7.949235776			
O	-5.812892566	10.228816875	7.965656125			
O	3.821761415	-0.068770629	7.936261826			
O	1.662732443	3.188254416	8.259075314			
O	-0.039258280	6.776446539	7.974234968			
O	-1.930954864	10.123025046	8.006137622			
O	7.865302321	-0.081304936	7.968604623			
O	5.790735561	2.054736727	9.125480391			
O	3.625668605	6.935326907	7.813035934			
O	1.899005107	10.152407947	7.975829100			
O	11.695251288	0.004988789	7.988005163			
O	10.317833860	3.074401580	8.355234207			
O	9.072630809	7.203518279	9.118755220			
O	5.839364475	10.513395901	8.322491995			
O	1.984298081	1.146331013	4.804391561			
O	-0.038764077	4.486800131	4.748082451			
O	-1.957009930	7.859243002	4.797144412			
O	-3.892449533	11.243563487	4.802247817			
O	5.851637078	1.107244970	4.784895042			
O	3.873176402	4.530119190	4.629945315			
O	1.925234395	7.888977955	4.790174500			
O	0.007856741	11.257696128	4.797602041			
O	9.701099872	1.131108238	4.827716924			
O	7.790079010	4.496389371	4.618488448			
O	5.806346334	7.872619833	4.627565011			
O	3.882266062	11.294166482	4.751954690			
O	13.643790996	1.114789941	4.793880325			
O	11.668858486	4.521400948	4.819643738			
O	9.757570206	7.877399961	4.782602858			
O	7.790138642	11.203026336	4.825040928			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.053634233	4.488988240	7.187894443			
Ce	-1.935072912	7.878675924	7.188661850			
Ce	-3.893318770	11.247006158	7.176629372			
Ce	5.840617623	0.978258831	7.309986936			
Ce	3.803752973	4.597538673	6.856650885			
Ce	1.799723955	7.969830751	7.140171508			
Ce	-0.001336115	11.243972710	7.191587864			
Ce	9.783688494	1.068661578	7.214652014			
Ce	7.794881648	4.517130120	6.840784566			
Ce	5.716361529	7.902946583	6.861113152			
Ce	3.878278090	11.311258781	7.196424290			
Ce	13.645458493	1.121745865	7.143432038			
Ce	11.774912836	4.497269833	7.204053907			
Ce	9.871642792	7.950699272	7.310751474			
Ce	7.810821844	11.283348870	7.208128573			
Ce	0.001485369	2.254146153	3.968686697			
Ce	-1.953580261	5.610460736	3.977948117			
Ce	-3.893459901	8.991840268	3.990708581			
Ce	-5.838687170	12.360414376	3.987271012			
Ce	3.909265386	2.215538055	3.965639239			
Ce	1.882304584	5.633449614	3.919001130			
Ce	-0.023281680	9.008406991	3.962845229			
Ce	-1.944100663	12.366704820	3.988653538			
Ce	7.783269127	2.204441676	3.958614515			
Ce	5.828734038	5.629799348	3.848590230			
Ce	3.853130443	9.048775207	3.920645656			
Ce	1.951866419	12.379983437	3.981506875			
Ce	11.673618504	2.252165613	3.978073594			
Ce	9.773278718	5.650028954	3.954170192			
Ce	7.825820390	9.002987976	3.978502172			
Ce	5.840842558	12.360207383	3.976946549			
Pt	7.328098569	6.421036369	9.268788124			
Pt	6.125446508	3.920497672	9.287228231			
Pt	3.303528754	3.910886315	9.309581710			
Pt	4.747413865	6.161357355	9.330957806			
Pt	8.790609760	4.024058980	9.250681034			
Pt	5.946608467	8.670982330	9.297136890			
Pt	4.579793583	4.510642131	11.360540237			
Pt	7.296604089	4.835975013	11.192002642			

Pt₉/CeO₂(111) – GM (0.0 eV)

153

O	0.019511866	-0.004212586	3.179323891			
O	-1.958945439	3.367418876	3.142968778			
O	-3.881566222	6.760837468	3.178623728			
O	-5.813140300	10.122765867	3.163196770			
O	3.897933910	-0.019135968	3.163563316			
O	1.924041619	3.350821416	3.143604811			
O	-0.030770683	6.738272128	3.149868153			
O	-1.957562429	10.122950457	3.167310713			
O	7.776797017	-0.011714947	3.180418291			
O	5.876403096	3.342180416	3.148045904			
O	3.898549668	6.743836743	3.095029192			
O	1.945763636	10.150921914	3.148890568			
O	11.683965978	0.025700948	3.143422210			
O	9.760557585	3.357591927	3.142653491			
O	7.836788477	6.727701514	3.146992975			
O	5.856783293	10.152827089	3.150610642			
O	-0.013190503	2.247486948	6.319907726			
O	-1.961953638	5.619165247	6.335688228			
O	-3.877392704	9.001501195	6.393744047			
O	-5.824690061	12.382885613	6.367975970			
O	3.910857939	2.376420781	6.446406203			
O	1.745911049	5.500855788	6.303987669			
O	0.114241091	8.916094522	6.469284009			
O	-1.934928231	12.351233223	6.378937972			
O	7.832696439	2.213384607	6.328991968			
O	6.088958965	5.486371783	6.296283724			
O	3.927317028	9.249842526	6.295516650			
O	1.954300167	12.389634758	6.339135772			
O	11.693091940	2.253296255	6.315023722			
O	9.783971261	5.616571717	6.333719029			
O	7.709919099	8.923201831	6.459746492			
O	5.856379105	12.398239631	6.332419889			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	0.030440774	0.017418961	7.943858621			
O	-2.013265824	3.335113527	7.968371159			
O	-3.866069682	6.772578312	7.972133134			
O	-5.803633962	10.152720122	7.976423571			
O	3.913039286	-0.010382663	7.957687554			
O	1.435621476	3.056451251	8.361901172			
O	-0.518843185	6.448569615	8.395057203			
O	-1.939982513	10.126570340	7.985087687			
O	7.778067970	-0.026805118	7.970217112			
O	6.429662889	3.009043534	8.396132503			
O	3.916402097	6.749104525	6.004906549			
O	1.946089458	10.679711759	8.355906376			
O	11.690378278	0.096841824	7.964013072			
O	9.835517988	3.322095259	7.963149658			
O	8.413289780	6.429829475	8.423222694			
O	5.886701498	10.742238018	8.390675330			
O	1.989667051	1.134077218	4.809896649			
O	-0.056299567	4.469963543	4.731099413			
O	-1.926537723	7.907795185	4.834215961			
O	-3.886577680	11.238149626	4.817864699			
O	5.814511203	1.109896925	4.828051670			
O	3.904806547	4.426560751	4.558449839			
O	1.898007552	7.909316808	4.570401921			
O	-0.013057149	11.202212378	4.835971368			
O	9.748163677	1.120640715	4.780944362			
O	7.871919399	4.449031461	4.731425990			
O	5.923400939	7.898461148	4.554686970			
O	3.902088208	11.319155226	4.731471320			
O	13.630257326	1.133903880	4.778334189			
O	11.689909446	4.496331478	4.781268198			
O	9.740866577	7.904618478	4.831019445			
O	7.821299800	11.211284725	4.831215276			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.140111352	4.424486257	7.216588415			
Ce	-1.981150805	7.881695761	7.220719481			
Ce	-3.885047914	11.252689548	7.180086601			
Ce	5.879406949	1.057608801	7.212154388			
Ce	3.920014962	4.632178891	6.771872213			
Ce	2.079487069	7.818420266	6.789485294			
Ce	-0.023744263	11.269467836	7.215331657			
Ce	9.750037728	1.119505306	7.128079113			
Ce	7.970905566	4.400465101	7.217454405			
Ce	5.759472028	7.803836922	6.775785490			
Ce	3.911643798	11.411355981	7.217396763			
Ce	13.636389169	1.132756745	7.126741078			
Ce	11.695800008	4.499369355	7.131818972			
Ce	9.810687004	7.883289999	7.220278588			
Ce	7.841144049	11.304605786	7.211079603			
Ce	-0.007565480	2.261545020	3.958900933			
Ce	-1.941385023	5.614327363	3.967789421			
Ce	-3.880774111	8.987843933	3.995350140			
Ce	-5.834351623	12.362547335	3.987144424			
Ce	3.907361330	2.195639308	3.948012596			
Ce	1.915949799	5.603365783	3.892302819			
Ce	-0.038022263	9.017081131	3.958598236			
Ce	-1.934936797	12.358782343	3.990315370			
Ce	7.808951705	2.244006753	3.969024907			
Ce	5.894056497	5.593712524	3.885562155			
Ce	3.905184295	9.035075628	3.889281615			
Ce	1.964317105	12.366942446	3.969656974			
Ce	11.685350264	2.250016130	3.953495055			
Ce	9.748421138	5.607615576	3.968151726			
Ce	7.850208076	9.018477393	3.956446192			
Ce	5.838940190	12.373295110	3.967002580			
Pt	6.634332520	6.756634613	9.278102201			
Pt	5.299457966	4.384025890	9.266810287			
Pt	2.603046739	4.334747698	9.214881497			
Pt	3.962624701	6.723680261	9.190772929			
Pt	2.596600878	9.028467185	9.284825038			
Pt	5.318772096	9.027371939	9.276171533			
Pt	1.238097843	6.735834020	9.259974035			
Pt	2.396045643	7.269114386	11.328512727			
Pt	3.715092284	4.924001570	11.239712390			

Pt₉/ CeO₂(111) – “Iso1_2D” (+0.01 eV)

153

O	0.020408535	-0.025127916	3.174075098			
O	-1.965356621	3.357416733	3.134607917			
O	-3.900985865	6.763908805	3.175620040			
O	-5.811002909	10.121301368	3.172957250			
O	3.904728085	-0.040912185	3.175196811			
O	1.926455574	3.335370951	3.143136514			
O	-0.042616331	6.738302120	3.145920445			
O	-1.970670196	10.129549755	3.177556111			
O	7.776176514	-0.008355521	3.167883849			
O	5.877203447	3.332538033	3.150259436			
O	3.911356394	6.749482536	3.083680249			
O	1.935691961	10.158527077	3.151909555			
O	11.685121745	0.025562304	3.136776708			
O	9.758442323	3.359725071	3.137801497			
O	7.844358866	6.749301755	3.156194883			
O	5.879649863	10.155589520	3.155198830			
O	0.005014793	2.220115208	6.310711407			
O	-1.969652756	5.606100664	6.328445094			
O	-3.837218768	9.040202745	6.497018234			
O	-5.732718342	12.372630130	6.471092692			
O	3.901411358	2.370245700	6.269808769			
O	1.733324780	5.487209355	6.283157628			
O	0.119082267	8.925884257	6.276925996			
O	-1.993372402	12.312660046	6.531743155			
O	7.832165100	2.236661733	6.331807760			
O	6.073851140	5.476864686	6.293617936			
O	3.891675494	9.252618653	6.292074198			
O	1.969114493	12.386711704	6.332306954			
O	11.691917119	2.244058290	6.287749454			
O	9.773339079	5.633117998	6.334464144			
O	7.685936116	8.918816438	6.498377500			
O	5.882896819	12.377798585	6.332447930			
O	1.945956000	1.123490000	0.001021000	0	0	0
O	-0.000006000	4.493961000	0.001121000	0	0	0
O	-1.946000000	7.864481000	0.000931000	0	0	0
O	-3.891953000	11.234965000	0.000876000	0	0	0
O	5.837850000	1.123506000	0.000808000	0	0	0
O	3.891925000	4.493984000	0.001009000	0	0	0
O	1.945969000	7.864460000	0.000941000	0	0	0
O	-0.000021000	11.234979000	0.000655000	0	0	0
O	9.729811000	1.123540000	0.000729000	0	0	0
O	7.783854000	4.494039000	0.000733000	0	0	0
O	5.837911000	7.864500000	0.000835000	0	0	0
O	3.891926000	11.234988000	0.000650000	0	0	0
O	13.621737000	1.123533000	0.000891000	0	0	0
O	11.675771000	4.494010000	0.000846000	0	0	0
O	9.729792000	7.864503000	0.000830000	0	0	0
O	7.783844000	11.234970000	0.000924000	0	0	0
O	0.000066000	2.247023000	1.598549000	0	0	0
O	-1.945920000	5.617441000	1.598583000	0	0	0

O	-3.891916000	8.987945000	1.598509000	0	0	0
O	-5.837929000	12.358604000	1.598550000	0	0	0
O	3.891780000	2.247055000	1.598517000	0	0	0
O	1.945983000	5.617420000	1.598591000	0	0	0
O	0.000013000	8.987938000	1.598556000	0	0	0
O	-1.946019000	12.358549000	1.598530000	0	0	0
O	7.783756000	2.246987000	1.598516000	0	0	0
O	5.837742000	5.617494000	1.598530000	0	0	0
O	3.891888000	8.987855000	1.598534000	0	0	0
O	1.945904000	12.358490000	1.598570000	0	0	0
O	11.675852000	2.247061000	1.598580000	0	0	0
O	9.729871000	5.617537000	1.598528000	0	0	0
O	7.783856000	8.987999000	1.598572000	0	0	0
O	5.837989000	12.358582000	1.598594000	0	0	0
O	0.034186422	-0.006841115	7.947279722			
O	-2.040037893	3.294222457	7.950595880			
O	-3.886263993	6.738657625	7.977391139			
O	-5.815782589	10.124217964	8.031443093			
O	3.919313090	0.124632319	8.229614899			
O	1.256107341	3.073726810	8.446409227			
O	-0.599635636	6.243525784	8.478187669			
O	-1.817129734	10.031812507	8.244244622			
O	7.829804944	0.009936102	7.965271342			
O	6.656152893	3.124847493	8.503271194			
O	3.903717044	6.742972201	5.998860613			
O	2.149715893	10.898997135	8.489440574			
O	11.719655918	0.123160004	7.953528180			
O	9.868444046	3.326257553	7.954092190			
O	8.402867240	6.434187086	8.480612859			
O	5.889969208	10.775597682	8.472886973			
O	1.967916591	1.079335342	4.801650861			
O	-0.066140318	4.454364951	4.702641802			
O	-1.979786233	7.885305202	4.829488396			
O	-3.887361474	11.220091681	4.869679719			
O	5.852806665	1.062932720	4.850042101			
O	3.904508761	4.452552410	4.528608959			
O	1.918473397	7.887309175	4.528559865			
O	-0.037652555	11.265896164	4.847243991			
O	9.743231967	1.123415589	4.774502394			
O	7.872285779	4.460900166	4.712873899			
O	5.917808839	7.907533783	4.559872741			
O	3.915514683	11.321490142	4.711641437			
O	13.634558053	1.119764660	4.774093261			
O	11.680820133	4.496025498	4.776827618			
O	9.755033591	7.932102568	4.876827404			
O	7.864015562	11.214435520	4.875497780			
Ce	0.000031000	0.000040000	0.792349000	0	0	0
Ce	-1.945945000	3.370493000	0.792321000	0	0	0
Ce	-3.891919000	6.740983000	0.792328000	0	0	0
Ce	-5.837868000	10.111488000	0.792349000	0	0	0
Ce	3.891860000	0.000037000	0.792334000	0	0	0
Ce	1.945970000	3.370480000	0.792306000	0	0	0
Ce	0.000032000	6.740937000	0.792438000	0	0	0
Ce	-1.945962000	10.111477000	0.792329000	0	0	0

Ce	7.783813000	-0.000028000	0.792315000	0	0	0
Ce	5.837791000	3.370514000	0.792343000	0	0	0
Ce	3.891908000	6.740957000	0.792337000	0	0	0
Ce	1.945932000	10.111469000	0.792321000	0	0	0
Ce	11.675799000	0.000013000	0.792407000	0	0	0
Ce	9.729828000	3.370538000	0.792349000	0	0	0
Ce	7.783832000	6.741001000	0.792346000	0	0	0
Ce	5.837884000	10.111477000	0.792366000	0	0	0
Ce	1.945933000	1.123513000	7.151559000	0	0	0
Ce	-0.158028621	4.385889312	7.203132643			
Ce	-1.986857585	7.797728473	7.211811558			
Ce	-3.903522127	11.213939244	7.255690498			
Ce	5.960592050	1.102528268	7.217178245			
Ce	3.899454784	4.621276263	6.744367192			
Ce	2.056419452	7.798902583	6.744578011			
Ce	0.051106129	11.313763889	7.212913172			
Ce	9.779953628	1.136814564	7.121073703			
Ce	7.995463684	4.434941216	7.212093314			
Ce	5.727292201	7.795596297	6.771847732			
Ce	3.956211165	11.432528474	7.211332121			
Ce	13.642808138	1.128314039	7.123483853			
Ce	11.694371521	4.474931761	7.126369879			
Ce	9.804903642	7.865066611	7.244414068			
Ce	7.836972020	11.304336045	7.242764890			
Ce	-0.008704622	2.244652893	3.945578774			
Ce	-1.951301981	5.607384927	3.950973348			
Ce	-3.880483959	8.990480831	4.004440079			
Ce	-5.820258864	12.351910243	3.996106902			
Ce	3.907446094	2.190415877	3.934009936			
Ce	1.907869002	5.592207691	3.871165837			
Ce	-0.043995098	9.016990366	3.944399898			
Ce	-1.939726452	12.353917584	4.006339154			
Ce	7.811435785	2.242005563	3.954822729			
Ce	5.894696104	5.597374435	3.877830479			
Ce	3.904905747	9.042961107	3.878159311			
Ce	1.960744154	12.375333696	3.954452715			
Ce	11.685203581	2.247128033	3.937274217			
Ce	9.747869577	5.607376937	3.956453587			
Ce	7.852715806	9.023021267	3.965087055			
Ce	5.844805215	12.373513013	3.953934686			
Pt	6.568885487	6.760937688	9.232749434			
Pt	5.219942409	4.349319490	9.206598817			
Pt	2.570948302	4.378126394	9.231405491			
Pt	3.871426154	6.706861490	9.213388199			
Pt	2.500386616	9.048808463	9.209199729			
Pt	5.260334141	9.022529036	9.232970569			
Pt	1.200201110	6.740148036	9.230519816			
Pt	-0.157917923	9.086053440	9.143154222			
Pt	3.923550639	2.029289881	9.143053879			

Pt₁₀/ CeO₂(111) – GM (0.0 eV)

154

O	0.019511866	-0.004212586	3.179323891			
O	-1.958945439	3.367418876	3.142968778			
O	-3.881566222	6.760837468	3.178623728			
O	-5.813140300	10.122765867	3.163196770			
O	3.897933910	-0.019135968	3.163563316			
O	1.924041619	3.350821416	3.143604811			
O	-0.030770683	6.738272128	3.149868153			
O	-1.957562429	10.122950457	3.167310713			
O	7.776797017	-0.011714947	3.180418291			
O	5.876403096	3.342180416	3.148045904			
O	3.898549668	6.743836743	3.095029192			
O	1.945763636	10.150921914	3.148890568			
O	11.683965978	0.025700948	3.143422210			
O	9.760557585	3.357591927	3.142653491			
O	7.836788477	6.727701514	3.146992975			
O	5.856783293	10.152827089	3.150610642			
O	-0.013190503	2.247486948	6.319907726			
O	-1.961953638	5.619165247	6.335688228			
O	-3.877392704	9.001501195	6.393744047			
O	-5.824690061	12.382885613	6.367975970			
O	3.910857939	2.376420781	6.446406203			
O	1.745911049	5.500855788	6.303987669			
O	0.114241091	8.916094522	6.469284009			
O	-1.934928231	12.351233223	6.378937972			
O	7.832696439	2.213384607	6.328991968			
O	6.088958965	5.486371783	6.296283724			
O	3.927317028	9.249842526	6.295516650			
O	1.954300167	12.389634758	6.339135772			
O	11.693091940	2.253296255	6.315023722			
O	9.783971261	5.616571717	6.333719029			
O	7.709919099	8.923201831	6.459746492			
O	5.856379105	12.398239631	6.332419889			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
O	9.729810481	1.123540270	0.000728614	0	0	0
O	7.783854129	4.494039180	0.000732727	0	0	0
O	5.837910993	7.864500108	0.000834859	0	0	0
O	3.891925883	11.234988599	0.000649737	0	0	0
O	13.621736258	1.123532495	0.000891287	0	0	0
O	11.675770307	4.494010663	0.000846015	0	0	0
O	9.729791529	7.864503147	0.000829781	0	0	0
O	7.783844501	11.234970236	0.000923532	0	0	0
O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

O	-3.891916014	8.987944574	1.598509327	0	0	0
O	-5.837928876	12.358604387	1.598549557	0	0	0
O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
O	7.783755910	2.246986911	1.598516049	0	0	0
O	5.837742513	5.617493850	1.598530420	0	0	0
O	3.891888148	8.987855029	1.598534342	0	0	0
O	1.945904088	12.358489995	1.598570511	0	0	0
O	11.675852231	2.247061321	1.598580371	0	0	0
O	9.729871219	5.617537303	1.598527510	0	0	0
O	7.783856593	8.987998806	1.598571536	0	0	0
O	5.837989493	12.358581803	1.598593568	0	0	0
O	0.030440774	0.017418961	7.943858621			
O	-2.013265824	3.335113527	7.968371159			
O	-3.866069682	6.772578312	7.972133134			
O	-5.803633962	10.152720122	7.976423571			
O	3.913039286	-0.010382663	7.957687554			
O	1.435621476	3.056451251	8.361901172			
O	-0.518843185	6.448569615	8.395057203			
O	-1.939982513	10.126570340	7.985087687			
O	7.778067970	-0.026805118	7.970217112			
O	6.429662889	3.009043534	8.396132503			
O	3.916402097	6.749104525	6.004906549			
O	1.946089458	10.679711759	8.355906376			
O	11.690378278	0.096841824	7.964013072			
O	9.835517988	3.322095259	7.963149658			
O	8.413289780	6.429829475	8.423222694			
O	5.886701498	10.742238018	8.390675330			
O	1.989667051	1.134077218	4.809896649			
O	-0.056299567	4.469963543	4.731099413			
O	-1.926537723	7.907795185	4.834215961			
O	-3.886577680	11.238149626	4.817864699			
O	5.814511203	1.109896925	4.828051670			
O	3.904806547	4.426560751	4.558449839			
O	1.898007552	7.909316808	4.570401921			
O	-0.013057149	11.202212378	4.835971368			
O	9.748163677	1.120640715	4.780944362			
O	7.871919399	4.449031461	4.731425990			
O	5.923400939	7.898461148	4.554686970			
O	3.902088208	11.319155226	4.731471320			
O	13.630257326	1.133903880	4.778334189			
O	11.689909446	4.496331478	4.781268198			
O	9.740866577	7.904618478	4.831019445			
O	7.821299800	11.211284725	4.831215276			
Ce	0.000030793	0.000040231	0.792348771	0	0	0
Ce	-1.945944948	3.370492589	0.792321265	0	0	0
Ce	-3.891919469	6.740982860	0.792327730	0	0	0
Ce	-5.837868276	10.111487965	0.792348924	0	0	0
Ce	3.891860121	0.000036876	0.792333612	0	0	0
Ce	1.945969646	3.370479767	0.792306289	0	0	0
Ce	0.000032378	6.740936664	0.792437995	0	0	0
Ce	-1.945962041	10.111476725	0.792329279	0	0	0

Ce	7.783812679	-0.000027545	0.792315061	0	0	0
Ce	5.837791112	3.370514467	0.792342945	0	0	0
Ce	3.891907982	6.740956664	0.792337239	0	0	0
Ce	1.945931595	10.111469724	0.792320593	0	0	0
Ce	11.675799156	0.000012720	0.792407333	0	0	0
Ce	9.729827943	3.370537627	0.792349346	0	0	0
Ce	7.783832251	6.741001247	0.792346177	0	0	0
Ce	5.837884575	10.111477045	0.792366343	0	0	0
Ce	1.945932653	1.123512509	7.151559344	0	0	0
Ce	-0.140111352	4.424486257	7.216588415			
Ce	-1.981150805	7.881695761	7.220719481			
Ce	-3.885047914	11.252689548	7.180086601			
Ce	5.879406949	1.057608801	7.212154388			
Ce	3.920014962	4.632178891	6.771872213			
Ce	2.079487069	7.818420266	6.789485294			
Ce	-0.023744263	11.269467836	7.215331657			
Ce	9.750037728	1.119505306	7.128079113			
Ce	7.970905566	4.400465101	7.217454405			
Ce	5.759472028	7.803836922	6.775785490			
Ce	3.911643798	11.411355981	7.217396763			
Ce	13.636389169	1.132756745	7.126741078			
Ce	11.695800008	4.499369355	7.131818972			
Ce	9.810687004	7.883289999	7.220278588			
Ce	7.841144049	11.304605786	7.211079603			
Ce	-0.007565480	2.261545020	3.958900933			
Ce	-1.941385023	5.614327363	3.967789421			
Ce	-3.880774111	8.987843933	3.995350140			
Ce	-5.834351623	12.362547335	3.987144424			
Ce	3.907361330	2.195639308	3.948012596			
Ce	1.915949799	5.603365783	3.892302819			
Ce	-0.038022263	9.017081131	3.958598236			
Ce	-1.934936797	12.358782343	3.990315370			
Ce	7.808951705	2.244006753	3.969024907			
Ce	5.894056497	5.593712524	3.885562155			
Ce	3.905184295	9.035075628	3.889281615			
Ce	1.964317105	12.366942446	3.969656974			
Ce	11.685350264	2.250016130	3.953495055			
Ce	9.748421138	5.607615576	3.968151726			
Ce	7.850208076	9.018477393	3.956446192			
Ce	5.838940190	12.373295110	3.967002580			
Pt	6.634332520	6.756634613	9.278102201			
Pt	5.299457966	4.384025890	9.266810287			
Pt	2.603046739	4.334747698	9.214881497			
Pt	3.962624701	6.723680261	9.190772929			
Pt	2.596600878	9.028467185	9.284825038			
Pt	5.318772096	9.027371939	9.276171533			
Pt	1.238097843	6.735834020	9.259974035			
Pt	2.396045643	7.269114386	11.328512727			
Pt	3.715092284	4.924001570	11.239712390			
Pt	5.271491754	7.321205850	11.483792237			

Pt₁₀/CeO₂(111) – “Iso1_2D” (+0.64 eV)

154

O	0.019689476	-0.005945147	3.159812543			
O	-1.961035815	3.359650741	3.129755875			
O	-3.886434650	6.753564025	3.159628809			
O	-5.803180113	10.127674278	3.172130340			
O	3.903088383	-0.034128844	3.170763763			
O	1.926937645	3.332123758	3.146692893			
O	-0.044356053	6.740347834	3.148007540			
O	-1.966926735	10.127539251	3.172817907			
O	7.779814779	-0.006307308	3.160287703			
O	5.874242869	3.329296681	3.147660515			
O	3.898510299	6.742159098	3.078219489			
O	1.930150173	10.158425711	3.149503676			
O	11.684177159	0.026420200	3.130453273			
O	9.759120803	3.358240454	3.130805098			
O	7.842500722	6.738925132	3.150105957			
O	5.868753713	10.159777017	3.149678976			
O	0.005488968	2.222077259	6.309710288			
O	-1.967181634	5.605434001	6.323864135			
O	-3.872945694	9.076408606	6.535419816			
O	-5.722511413	12.325701698	6.511468439			
O	3.904429628	2.367565540	6.269466929			
O	1.739443826	5.491302591	6.289033673			
O	0.115667628	8.924141574	6.272738291			
O	-2.005091432	12.306736590	6.532957177			
O	7.836842459	2.217573730	6.321847482			
O	6.083806585	5.490515557	6.292438734			
O	3.909410673	9.254463160	6.289939593			
O	1.953470482	12.399500606	6.322696039			
O	11.699000361	2.247634655	6.288680944			
O	9.785339492	5.607260738	6.320863931			
O	7.699395726	8.922067266	6.277470124			
O	5.866218264	12.404713767	6.320435572			
O	1.945956038	1.123490095	0.001020734	0	0	0
O	-0.000006047	4.493960919	0.001120585	0	0	0
O	-1.946000165	7.864480845	0.000931343	0	0	0
O	-3.891953031	11.234965363	0.000875751	0	0	0
O	5.837849536	1.123506072	0.000808031	0	0	0
O	3.891924611	4.493983954	0.001008664	0	0	0
O	1.945968863	7.864460661	0.000940862	0	0	0
O	-0.000021389	11.234978713	0.000655464	0	0	0
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O	3.891925883	11.234988599	0.000649737	0	0	0
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O	0.000066191	2.247022839	1.598548591	0	0	0
O	-1.945919698	5.617440872	1.598583110	0	0	0

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O	3.891779667	2.247055153	1.598517312	0	0	0
O	1.945982536	5.617420162	1.598590681	0	0	0
O	0.000013276	8.987937580	1.598555755	0	0	0
O	-1.946018522	12.358549225	1.598529683	0	0	0
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O	7.783856593	8.987998806	1.598571536	0	0	0
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O	0.030299308	0.013017305	7.933957933			
O	-2.038506363	3.297473108	7.956385410			
O	-3.871557663	6.726041942	7.958249035			
O	-5.924227429	10.068626614	8.244389711			
O	3.926380508	0.133927203	8.243222210			
O	1.254809661	3.096815223	8.453579966			
O	-0.579405073	6.226707437	8.484780680			
O	-1.791470330	10.029928856	8.250608822			
O	7.818811806	0.001449881	7.960937147			
O	6.629920865	3.083941834	8.495767414			
O	3.909941178	6.746978030	6.022645969			
O	2.105525229	10.879827591	8.471534992			
O	11.699830435	0.142214092	7.958716363			
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O	8.438552736	6.227981589	8.496928240			
O	5.731437858	10.904335105	8.486209315			
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O	-0.064835945	4.455127357	4.704408657			
O	-1.994481209	7.889899486	4.839718993			
O	-3.877695649	11.229085074	4.867037076			
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O	-0.039915256	11.270492557	4.840277556			
O	9.752113090	1.128462820	4.769249630			
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O	11.687479124	4.486532257	4.770380011			
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Pt₁₀/CeO₂(111) – “Iso2_3D” (+1.03 eV)

154

O	0.014658879	-0.006706130	3.175976291			
O	-1.965212810	3.366142791	3.160173228			
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O	7.783840000	11.234970000	0.000920000	0	0	0
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Ce	-0.003250553	11.245373326	7.193067286			
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