

Electronic Supplementary Information: A Hybrid-DFT Investigation of Ce Oxidation State Upon Adsorption of F, Na, Ni, Pd and Pt on the $(\text{CeO}_2)_6$ Cluster

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1 Introduction

At the present electronic supporting information, we report several complementary data to support our statements, namely, *(i)* the calculated relative total energies for the $(\text{CeO}_2)_6$ clusters, *(ii)* tables with the structural, energetic, and electronic properties for all adsorption configurations calculated in this work, *(iii)* additional figures for the density of states, etc, and finally, *(iv)* the atomic positions of the five representative configurations selected with k-means algorithm.

2 Calculated Configurations for the $(\text{CeO}_2)_6$ Clusters

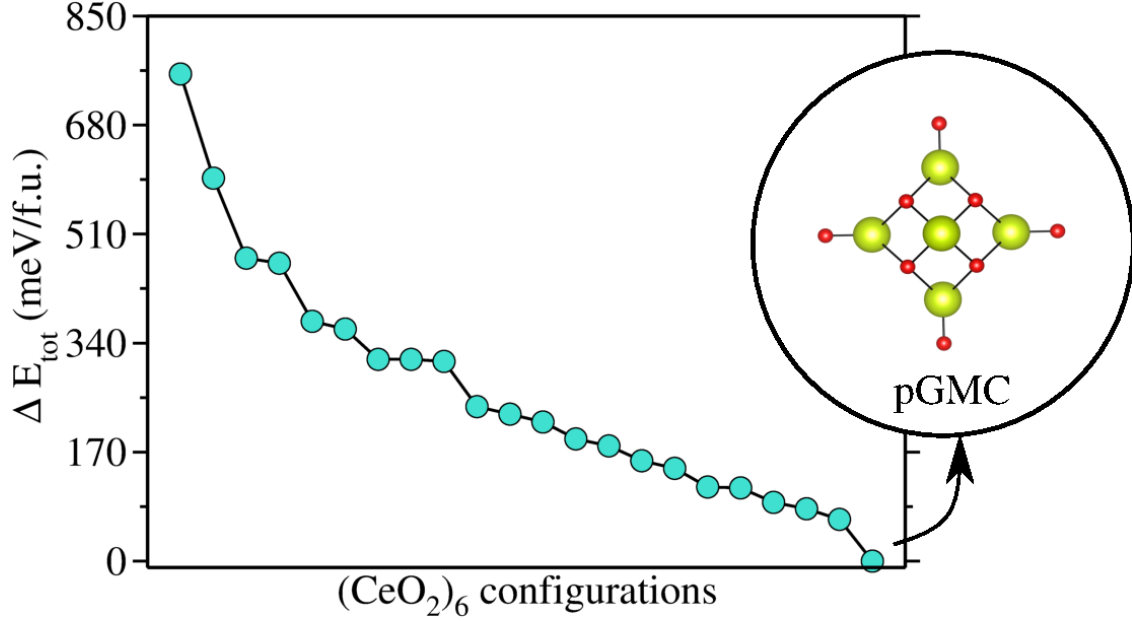


Figure 1: Calculated DFT-HSE06 configurations for the $(\text{CeO}_2)_6$ clusters. The putative global minimum configuration (pGMC) of $(\text{CeO}_2)_6$ clusters is highlighted in the sketch, which was employed as support for the adsorption of F, Na, Ni, Pd and Pt in this study.

Table 1: Results for the F/ Ce_2O_{12} configurations. Relative total energy, ΔE_{tot} , adsorption energy, E_{ad} , HOMO-LUMO energy separation, E_g , total magnetic moment, m_{tot} , smallest distance between adatom and the oxygen, d^{M-O} , and cerium ions, d^{M-Ce} , percentage change of the average bond lengths and coordination number of the four-fold cerium cations, $\Delta d_{av}^{Ce,CN4}$ and ΔCe^{CN4} , five-fold/one-fold cerium and oxygen ions, $\Delta d_{av}^{Ce,CN5}$, $\Delta d_{av}^{O,CN1}$, ΔCe^{CN5} , ΔO^{CN1} , and the centered oxygen anions, $\Delta d_{av}^{O,CN3}$ and ΔO^{CN3} , in relation to the non-adsorbed cluster.

ΔE_{tot} (eV)	E_{ad} (eV)	E_g (eV)	m_{tot} (μ_B)	d^{M-O} (\AA)	d^{M-Ce} (\AA)	$\Delta d_{av}^{Ce,CN4}$ (%)	$\Delta d_{av}^{Ce,CN5}$ (%)	$\Delta d_{av}^{O,CN1}$ (%)	$\Delta d_{av}^{O,CN3}$ (%)	ΔCe^{CN4} (%)	ΔCe^{CN5} (%)	ΔO^{CN1} (%)	ΔO^{CN3} (%)
2.50	-0.44	3.49	1.00	1.99	3.81	0.03	-0.12	0.30	-0.17	0.00	0.00	0.00	0.00
1.54	-1.39	2.31	1.00	1.78	2.17	0.22	0.42	-0.27	-1.62	0.00	-5.00	0.00	-14.58
1.49	-1.44	2.06	1.00	2.10	2.43	-0.57	1.62	-0.37	-0.18	0.00	0.00	0.00	-4.17
0.69	-2.25	3.24	1.00	2.92	2.06	-0.04	0.40	8.42	-0.32	0.00	0.00	25.00	2.08
0.69	-2.25	3.25	1.00	2.91	2.06	-0.04	0.40	8.42	-0.32	0.00	0.00	25.00	2.08
0.69	-2.25	3.24	1.00	2.91	2.06	-0.04	0.40	8.33	-0.32	0.00	0.00	25.00	2.08
0.41	-2.53	1.54	1.00	3.55	2.07	3.09	0.10	-0.28	0.80	0.00	0.00	0.00	0.00
0.41	-2.53	1.55	1.00	3.55	2.07	3.08	0.10	-0.28	0.80	0.00	0.00	0.00	0.00
0.41	-2.53	1.55	1.00	3.55	2.07	3.08	0.11	-0.29	0.80	0.00	0.00	0.00	0.00
0.00	-2.93	1.76	1.00	3.62	2.07	2.47	-0.92	2.79	-0.35	0.00	0.00	0.00	0.00
0.00	-2.94	1.76	1.00	3.62	2.07	2.47	-0.93	2.76	-0.35	0.00	0.00	0.00	0.00

Table 2: Results for the Na/(CeO₂)₆ configurations. Relative total energy, ΔE_{tot} , adsorption energy, E_{ad} , HOMO-LUMO energy separation, E_g , total magnetic moment, m_{tot} , smallest distance between adatom and the oxygen, d^{M-O} , and cerium ions, d^{M-Ce} , percentage change of the average bond lengths and coordination number of the four-fold cerium cations, $\Delta d_{av}^{Ce,CN4}$, and ΔCe^{CN4} , five-fold/one-fold cerium/oxygen ions, $\Delta d_{av}^{Ce,CN5}$, $\Delta d_{av}^{O,CN1}$, and ΔCe^{CN5} , ΔO^{CN1} , and the centered oxygen anions, $\Delta d_{av}^{O,CN3}$ and ΔO^{CN3} , in relation to the non-adsorbed cluster.

ΔE_{tot} (eV)	E_{ad} (eV)	E_g (eV)	m_{tot} (μ_B)	d^{M-O} (Å)	d^{M-Ce} (Å)	$\Delta d_{av}^{Ce,CN4}$ (%)	$\Delta d_{av}^{Ce,CN5}$ (%)	$\Delta d_{av}^{O,CN1}$ (%)	$\Delta d_{av}^{O,CN3}$ (%)	ΔCe^{CN4} (%)	ΔCe^{CN5} (%)	ΔO^{CN1} (%)	ΔO^{CN3} (%)
0.74	-2.25	1.92	1.00	2.04	3.99	3.40	-0.72	2.96	0.62	0.00	0.00	0.00	0.00
0.74	-2.25	1.91	1.00	2.04	3.99	3.39	-0.72	2.98	0.62	0.00	0.00	0.00	0.00
0.07	-2.92	1.91	1.00	2.29	3.23	3.39	-0.76	2.63	0.53	0.00	0.00	0.00	0.00
0.03	-2.96	1.95	1.00	2.29	3.23	3.38	-0.75	2.63	0.55	0.00	0.00	0.00	0.00
0.03	-2.96	1.95	1.00	2.29	3.23	3.37	-0.76	2.63	0.54	0.00	0.00	0.00	0.00
0.03	-2.96	1.96	1.00	2.29	3.23	3.38	-0.76	2.62	0.55	0.00	0.00	0.00	0.00
0.03	-2.96	1.95	1.00	2.29	3.23	3.38	-0.76	2.63	0.56	0.00	0.00	0.00	0.00
0.03	-2.96	1.95	1.00	2.29	3.23	3.37	-0.75	2.63	0.55	0.00	0.00	0.00	0.00
0.03	-2.96	1.96	1.00	2.29	3.23	3.37	-0.75	2.63	0.55	0.00	0.00	0.00	0.00
0.03	-2.96	1.95	1.00	2.29	3.23	3.37	-0.75	2.62	0.55	0.00	0.00	0.00	0.00
0.00	-2.99	2.08	1.00	2.28	3.23	3.44	-0.76	2.63	0.53	0.00	0.00	0.00	0.00

Table 3: Results for the Ni/(CeO₂)₆ configurations. Relative total energy, ΔE_{tot} , adsorption energy, E_{ad} , HOMO-LUMO energy separation, E_g , total magnetic moment, m_{tot} , smallest distance between adatom and the oxygen, d^{M-O} , and cerium ions, d^{M-Ce} , percentage change of the average bond lengths and coordination number of the four-fold cerium cations, $\Delta d_{av}^{Ce,CN4}$ and ΔCe^{CN4} , five-fold, one-fold cerium and oxygen ions, $\Delta d_{av}^{Ce,CN5}$, $\Delta d_{av}^{O,CN1}$ and ΔCe^{CN5} , ΔO^{CN1} , and the centered oxygen anions, $\Delta d_{av}^{O,CN3}$ and ΔO^{CN3} , in relation to the non-adsorbed cluster.

ΔE_{tot} (eV)	E_{ad} (eV)	E_g (eV)	m_{tot} (μ_B)	d^{M-O} (Å)	d^{M-Ce} (Å)	$\Delta d_{av}^{Ce,CN4}$ (%)	$\Delta d_{av}^{Ce,CN5}$ (%)	$\Delta d_{av}^{O,CN1}$ (%)	$\Delta d_{av}^{O,CN3}$ (%)	ΔCe^{CN4} (%)	ΔCe^{CN5} (%)	ΔO^{CN1} (%)	ΔO^{CN3} (%)
1.50	-1.88	1.91	0.00	1.85	2.51	0.85	-1.77	-0.17	-0.03	0.00	-15.00	0.00	-14.58
1.16	-2.22	1.14	0.00	1.83	3.04	0.01	0.73	-0.12	0.60	0.00	0.00	0.00	0.00
0.73	-2.65	1.64	0.00	1.83	2.84	2.12	-0.04	0.16	0.76	0.00	0.00	0.00	0.00
0.73	-2.65	1.63	0.00	1.83	2.84	2.13	-0.03	0.18	0.76	0.00	0.00	0.00	0.00
0.73	-2.65	1.63	0.00	1.83	2.84	2.11	-0.04	0.17	0.75	0.00	0.00	0.00	0.00
0.73	-2.65	1.63	0.00	1.83	2.84	2.12	-0.04	0.17	0.76	0.00	0.00	0.00	0.00
0.73	-2.65	1.63	0.00	1.83	2.84	2.12	-0.03	0.18	0.76	0.00	0.00	0.00	0.00
0.58	-2.80	1.75	0.00	1.78	2.61	3.53	-0.76	4.04	0.33	0.00	0.00	0.00	0.00
0.58	-2.80	1.75	0.00	1.78	2.61	0.91	-0.31	1.78	-1.19	0.00	-5.00	0.00	-10.42
0.58	-2.80	1.75	0.00	1.78	2.61	0.90	-0.29	1.79	-1.19	0.00	-5.00	0.00	-10.42
0.12	-3.26	1.51	0.00	1.77	3.79	3.55	-0.76	3.74	0.40	0.00	0.00	0.00	0.00
0.00	-3.38	1.59	2.00	1.74	3.79	3.53	-0.76	4.04	0.33	0.00	0.00	0.00	0.00

Table 4: Systematic calculations for the Ni/(CeO₂)₆ system with different initial magnetic configurations. Configuration label (only for calculation control), initial local magnetic moment for each specie (all atoms of the same specie or different values are indicated), total energy, E_{tot} , final local magnetic moment for each specie, and total magnetic moment for the Ni/(CeO₂)₆ system, m_{tot} . E_{tot} , local magnetic moments, and m_{tot} were obtained upon geometric optimizations. For the configurations without the indication of the initial local magnetic moment, we employed the magnetic configurations provided by the FHI-aims package via Hund’s rule. Only one of the six Ce atoms have local magnetic moment upon geometric optimization, which is indicated below, while the remaining 5 Ce atoms have a local magnetic moment of zero μ_B .

i	Initial local moment (μ_B)			E_{tot} (eV)	Final local moment (μ_B)			m_{tot} (μ_B)
	Ni	Ce	O		Ni	Ce	O	
8	2.00	-1.00	0.00	-1 539 291.263 877 98	0.00	0.00	0.00	0.00
8				-1 539 291.264 195 26				0.00
1	2.00	-1.00	0.00	-1 539 291.608 937 49	0.10	-0.18	0.08	0.00
1				-1 539 291.609 013 35				0.00
10				-1 539 291.748 287 29				0.00
11	2.00	-1.00	0.00	-1 539 292.033 229 81	0.52	-0.64	0.12	0.00
11				-1 539 292.033 236 45				0.00
5	2.00	-1.00	0.00	-1 539 292.033 443 16	0.53	-0.65	0.12	0.00
5				-1 539 292.033 453 29				0.00
12				-1 539 292.033 543 80				0.00
12	2.00	-1.00	0.00	-1 539 292.033 562 24	0.53	-0.65	0.12	0.00
10	2.00	-1.00	0.00	-1 539 292.034 008 89	0.53	-0.65	0.12	0.00
9				-1 539 292.034 619 83				0.00
9	2.00	-1.00	0.00	-1 539 292.034 634 71	0.52	-0.64	0.12	0.00
4				-1 539 292.184 053 98				0.00
4	2.00	-1.00	0.00	-1 539 292.184 056 83	0.00	0.00	0.00	0.00
6				-1 539 292.185 444 60				0.00
6	2.00	-1.00	0.00	-1 539 292.033 562 24	0.00	0.00	0.00	0.00
2	2.00	-1.00	0.00	-1 539 292.185 531 92	0.00	0.00	0.00	0.00
2				-1 539 292.185 532 67				0.00
7				-1 539 292.573 212 31				0.00
3	-1.00	1.00	0.00	-1 539 292.617 885 60	-1.02	1.03	-0.01	0.00
3	1.00	-1, 0, 0, 0, -1, 0	0.00	-1 539 292.617 910 67	-1.02	1.03	-0.01	0.00
3	1.00	-1, 0, 0, -1, 0, 0	0.00	-1 539 292.618 091 93	1.02	-1.02	0.00	0.00
7	1.00	-1, 0, -1, 0, 0, 0	0.00	-1 539 292.643 608 57	1.02	-1.02	0.00	0.00
7	2.00	-1.00	0.00	-1 539 292.648 016 59	1.02	-1.02	0.00	0.00
3				-1 539 292.765 708 13				2.00

Table 5: Results for the Pd/(CeO₂)₆ configurations. Relative total energy, ΔE_{tot} , adsorption energy, E_{ad} , HOMO-LUMO energy separation, E_g , total magnetic moment, m_{tot} , smallest distance between adatom and the oxygen, d^{M-O} , and cerium ions, d^{M-Ce} , percentage change of the average bond lengths and coordination number of the four-fold cerium cations, $\Delta d_{av}^{Ce,CN4}$ and ΔCe^{CN4} , five-fold/one-fold cerium/oxygen ions, $\Delta d_{av}^{Ce,CN5}$, $\Delta d_{av}^{O,CN1}$ and ΔCe^{CN5} , ΔO^{CN1} , and the centered oxygen anions, $\Delta d_{av}^{O,CN3}$ and ΔO^{CN3} , in relation to the non-adsorbed cluster.

ΔE_{tot} (eV)	E_{ad} (eV)	E_g (eV)	m_{tot} (μ_B)	d^{M-O} (\AA)	d^{M-Ce} (\AA)	$\Delta d_{av}^{Ce,CN4}$ (%)	$\Delta d_{av}^{Ce,CN5}$ (%)	$\Delta d_{av}^{O,CN1}$ (%)	$\Delta d_{av}^{O,CN3}$ (%)	ΔCe^{CN4} (%)	ΔCe^{CN5} (%)	ΔO^{CN1} (%)	ΔO^{CN3} (%)
0.56	-0.65	2.99	0.00	2.04	2.86	1.72	-1.14	-0.20	-1.34	0.00	-10.00	0.00	-16.67
0.25	-0.95	1.26	0.00	2.05	3.03	0.00	0.01	1.08	-0.15	0.00	0.00	0.00	0.00
0.25	-0.95	1.28	0.00	2.04	3.02	-0.01	0.03	1.09	-0.13	0.00	0.00	0.00	0.00
0.19	-1.01	2.26	0.00	2.04	3.06	-0.03	0.52	-0.05	0.35	0.00	0.00	0.00	0.00
0.19	-1.01	2.29	0.00	2.04	3.11	-0.05	0.54	-0.06	0.39	0.00	0.00	0.00	0.00
0.06	-1.14	2.35	0.00	2.04	2.89	1.11	-1.65	1.39	-3.56	0.00	-10.00	0.00	-16.67
0.00	-1.20	2.56	0.00	2.07	2.83	1.07	0.01	0.01	0.33	0.00	0.00	0.00	0.00
0.00	-1.20	2.56	0.00	2.06	2.83	-0.65	1.17	0.21	1.68	0.00	11.11	0.00	20.00
0.00	-1.20	2.55	0.00	2.06	2.84	1.06	0.01	0.01	0.33	0.00	0.00	0.00	0.00
0.00	-1.20	2.53	0.00	2.06	2.85	1.05	0.01	0.00	0.31	0.00	0.00	0.00	0.00
0.00	-1.20	2.55	0.00	2.06	2.84	1.07	0.00	0.01	0.33	0.00	0.00	0.00	0.00
0.00	-1.20	2.56	0.00	2.06	2.83	1.08	0.02	0.00	0.33	0.00	0.00	0.00	0.00
0.00	-1.20	2.58	0.00	2.07	2.82	1.08	0.01	0.01	0.34	0.00	0.00	0.00	0.00

Table 6: Results for the Pt/(CeO₂)₆ configurations. Relative total energy, ΔE_{tot} , adsorption energy, E_{ad} , HOMO-LUMO energy separation, E_g , total magnetic moment, m_{tot} , smallest distance between adatom and the oxygen, d^{M-O} , and cerium ions, d^{M-Ce} , percentage change of the average bond lengths and coordination number of the four-fold cerium cations, $\Delta d_{av}^{Ce,CN4}$ and ΔCe^{CN4} , five-fold and one-fold cerium and oxygen ions, $\Delta d_{av}^{Ce,CN5}$, $\Delta d_{av}^{O,CN1}$ and ΔCe^{CN5} , ΔO^{CN1} , and the centered oxygen anions, $\Delta d_{av}^{O,CN3}$ and ΔO^{CN3} , in relation to the non-adsorbed cluster.

ΔE_{tot} (eV)	E_{ad} (eV)	E_g (eV)	m_{tot} (μ_B)	d^{M-O} (\AA)	d^{M-Ce} (\AA)	$\Delta d_{av}^{Ce,CN4}$ (%)	$\Delta d_{av}^{Ce,CN5}$ (%)	$\Delta d_{av}^{O,CN1}$ (%)	$\Delta d_{av}^{O,CN3}$ (%)	ΔCe^{CN4} (%)	ΔCe^{CN5} (%)	ΔO^{CN1} (%)	ΔO^{CN3} (%)
2.36	-0.93	0.84	2.00	4.07	3.23	0.27	-0.03	0.14	0.11	0.00	0.00	0.00	0.00
2.36	-0.93	0.90	2.00	3.87	3.21	0.29	-0.03	0.13	0.12	0.00	0.00	0.00	0.00
0.96	-2.32	1.65	0.00	1.92	2.82	0.00	0.12	2.47	-0.28	0.00	0.00	0.00	0.00
0.96	-2.33	1.66	0.00	1.93	2.82	0.00	0.14	2.46	-0.26	0.00	0.00	0.00	0.00
0.95	-2.33	1.68	0.00	1.93	2.81	-0.01	0.15	2.49	-0.26	0.00	0.00	0.00	0.00
0.90	-2.39	2.67	0.00	1.93	3.10	-0.07	1.03	-0.21	-0.14	0.00	0.00	0.00	-4.17
0.61	-2.68	2.83	0.00	1.94	2.78	1.76	0.10	-0.12	0.60	0.00	0.00	0.00	0.00
0.60	-2.68	2.84	0.00	1.94	2.78	1.50	0.13	-0.26	0.49	0.00	0.00	0.00	0.00
0.60	-2.68	2.84	0.00	1.94	2.78	1.77	0.09	-0.12	0.59	0.00	0.00	0.00	0.00
0.60	-2.68	2.84	0.00	1.94	2.78	1.77	0.10	-0.12	0.59	0.00	0.00	0.00	0.00
0.48	-2.80	2.97	0.00	2.00	2.89	2.33	-0.99	-0.24	-1.04	0.00	-10.00	0.00	-16.67
0.00	-3.28	2.17	0.00	2.00	2.81	1.29	-1.45	2.06	-3.38	0.00	-10.00	0.00	-16.67

3 Projected Density of States

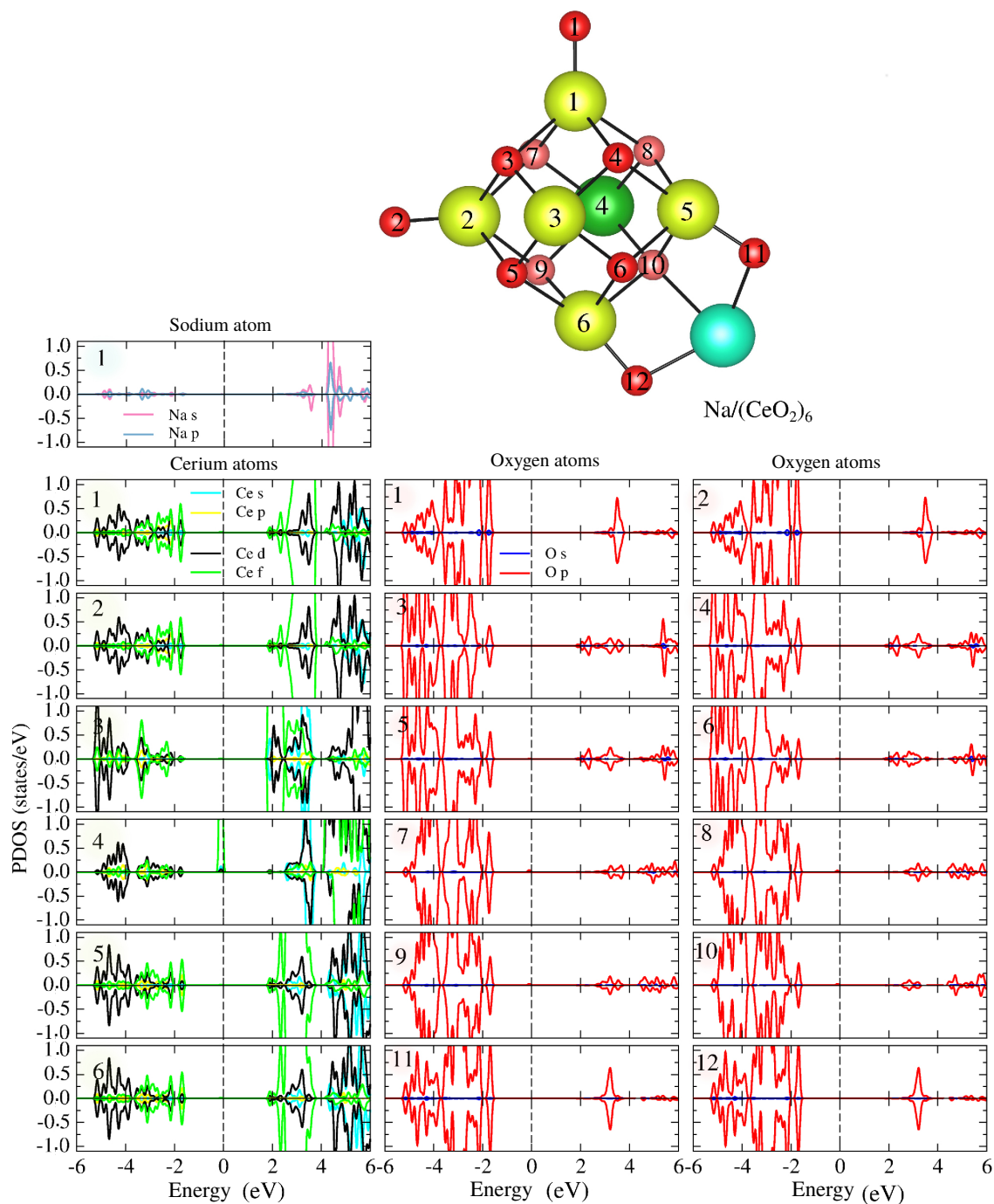


Figure 2: Projected density of states (PDOS) per species for the strongest adsorption of Na on the (CeO₂)₆ cluster. The numbers in the top-left side of PDOS plots indicates the number of ions in the Na/(CeO₂)₆ picture. The PDOS for the Ce number 4 clearly indicates a localized Ce-*f* state at the HOMO level.

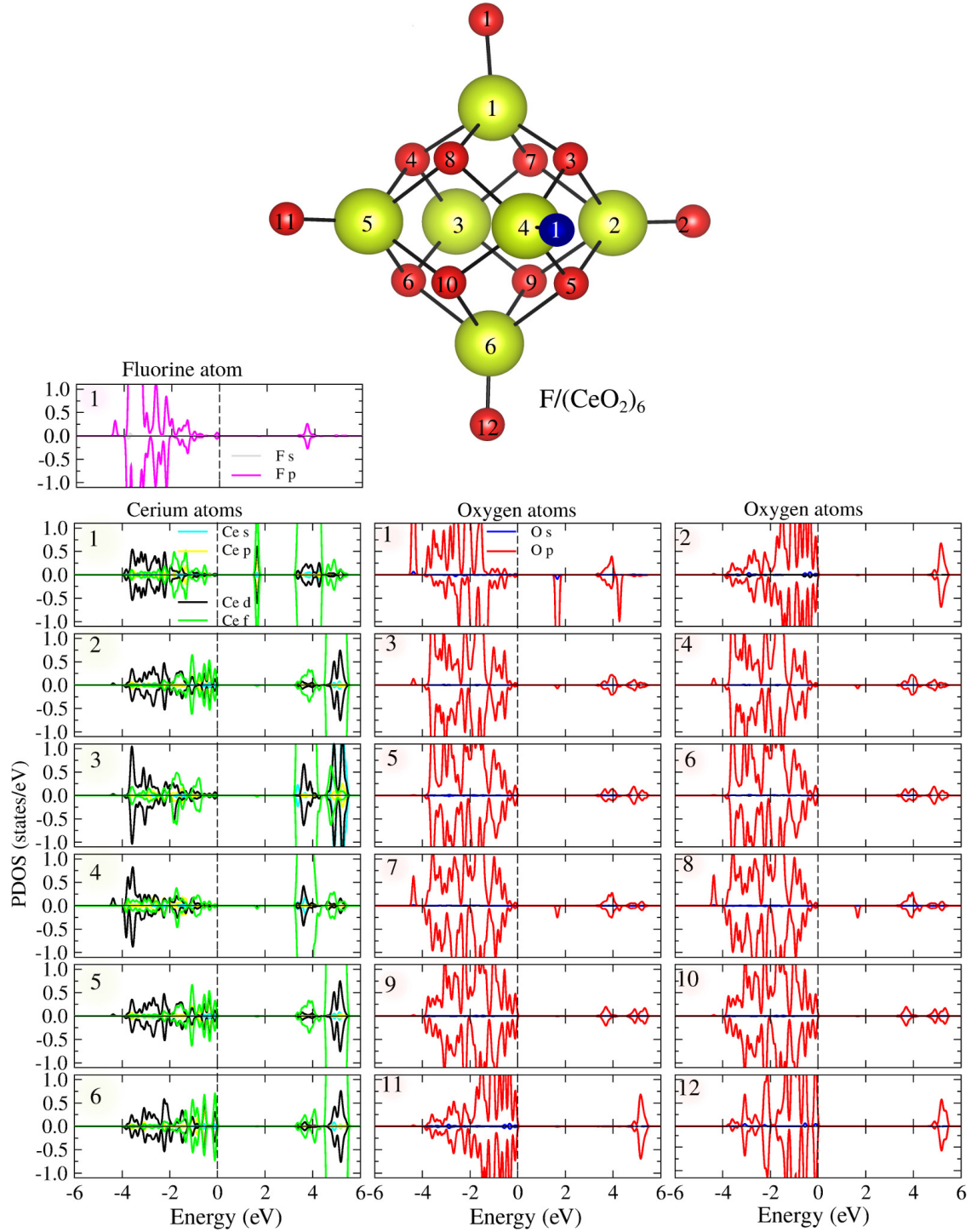


Figure 3: Projected density of states per species for the strongest adsorption of F on the $(\text{CeO}_2)_6$ cluster. The numbers in the top-left side of PDOs plots indicates the number of ions in the $\text{F}/(\text{CeO}_2)_6$ picture. The PDOs for the O number 1 clearly indicates a hole with O-*p* character.

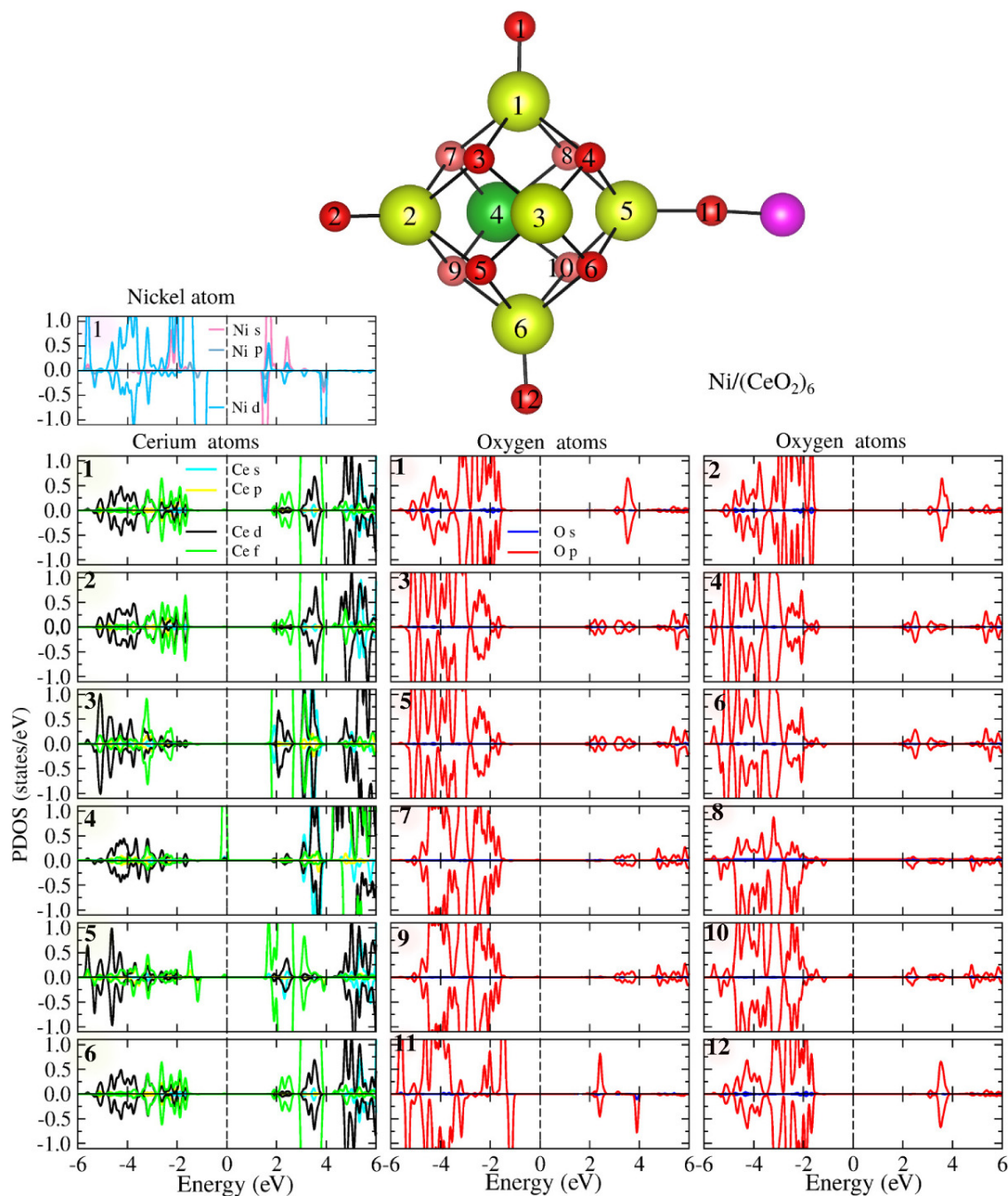


Figure 4: Projected density of states per species for the strongest adsorption of Ni on the (CeO₂)₆ cluster. The numbers in the top-left side of PDOs plots indicates the number of ions in the Ni/(CeO₂)₆ picture. The PDOs indicates the existence of an unpaired electron in the Ce–O–Ni moiety in addition to a localized Ce-*f* state at the HOMO level.

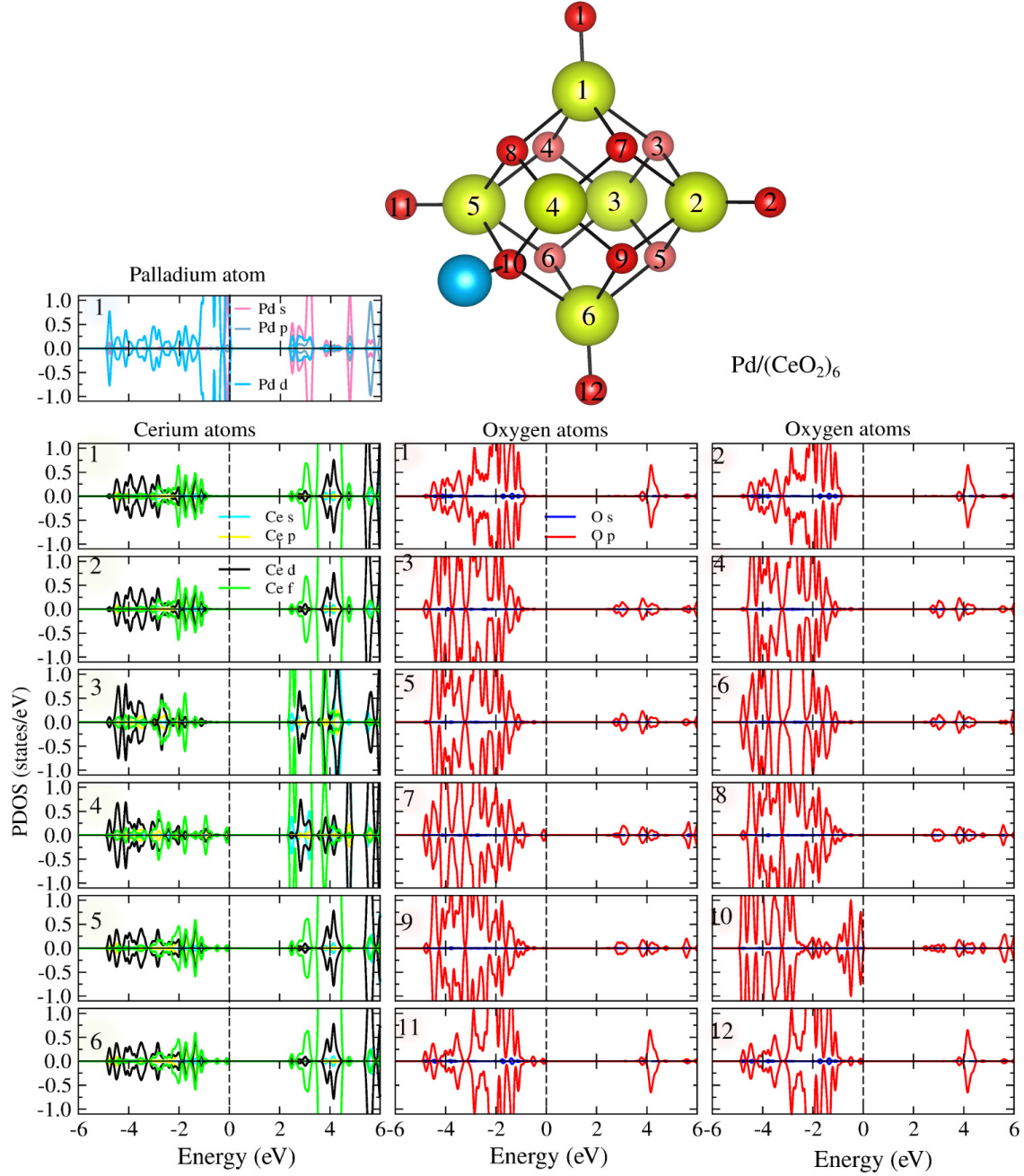


Figure 5: Projected density of states per species for the strongest adsorption of Pd on the (CeO₂)₆ cluster. Differently of the Na/(CeO₂)₆ and Ni/(CeO₂)₆ systems, no localized Ce-*f* states occurs at HOMO level of Pd/(CeO₂)₆.

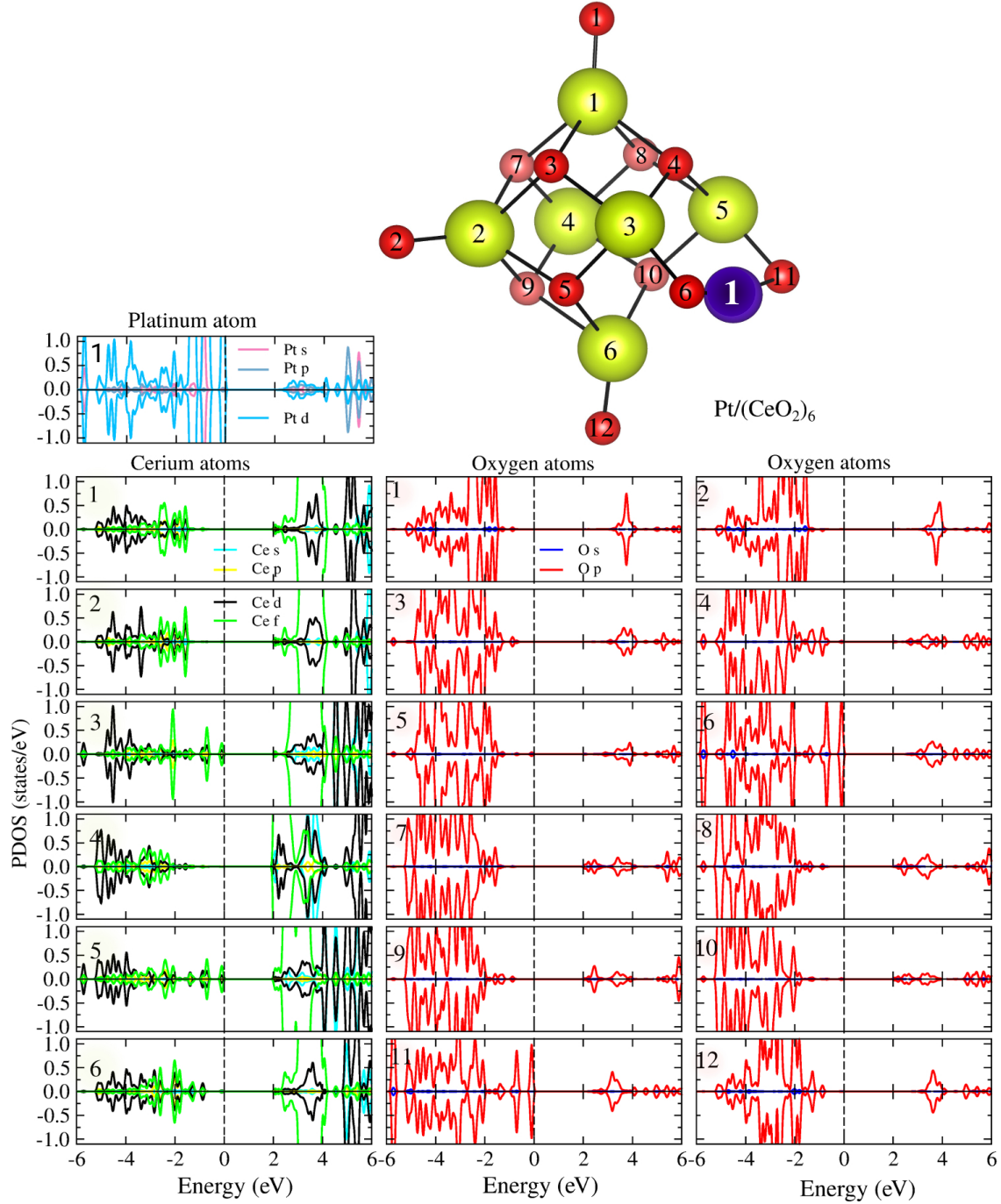


Figure 6: Projected density of states per species for the strongest adsorption of Pt on the (CeO₂)₆ cluster. Differently of the Na/(CeO₂)₆ and Ni/(CeO₂)₆ systems, no localized Ce-*f* states occurs at HOMO level of Pt/(CeO₂)₆.

4 Atomic Positions of the Five Lowest Energy Configurations for F, Na, Ni, Pd, Pt on the $(\text{CeO}_2)_6$ Cluster

Table 7: F/ $(\text{CeO}_2)_6$, $\Delta E_{tot} = 2.50$ eV and $E_{ad} = -0.44$ eV.

F	-6.053 388 000 000 000 0	-0.148 184 000 000 000 0	0.924 401 000 000 000 0
Ce	0.339 700 000 000 000 0	-2.327 329 000 000 000 2	-0.051 867 000 000 000 0
Ce	0.821 306 000 000 000 0	0.009 600 000 000 000 0	2.596 216 000 000 000 1
Ce	0.338 666 000 000 000 0	2.342 213 000 000 000 1	-0.052 051 000 000 000 0
Ce	-2.280 103 000 000 000 0	0.006 803 000 000 000 0	0.425 375 000 000 000 0
Ce	2.979 191 000 000 000 1	0.008 182 000 000 000 0	-0.535 582 000 000 000 0
Ce	-0.147 926 000 000 000 0	0.008 506 000 000 000 0	-2.699 815 000 000 000 1
O	1.879 693 000 000 000 1	-1.409 060 999 999 999 9	1.017 892 999 999 999 9
O	-0.739 981 000 000 000 0	1.413 589 000 000 000 0	1.490 269 000 000 000 1
O	1.140 004 000 000 000 0	0.009 220 000 000 000 0	4.353 606 000 000 000 1
O	1.401 539 000 000 000 1	1.425 861 000 000 000 0	-1.598 335 000 000 000 1
O	-1.215 127 000 000 000 1	-1.396 349 000 000 000 1	-1.112 374 999 999 999 9
O	-0.738 667 000 000 000 0	-1.396 090 000 000 000 1	1.489 935 000 000 000 0
O	-1.215 831 000 000 000 1	1.412 887 999 999 999 9	-1.113 888 000 000 000 0
O	1.401 731 000 000 000 1	-1.409 813 000 000 000 0	-1.597 351 000 000 000 0
O	-4.071 728 000 000 000 2	0.007 148 000 000 000 0	0.754 995 000 000 000 0
O	-0.457 430 000 000 000 0	0.011 100 000 000 000 0	-4.458 705 000 000 000 1
O	4.737 965 000 000 000 0	0.005 153 000 000 000 0	-0.850 187 000 000 000 0
O	1.880 379 999 999 999 9	1.426 557 000 000 000 1	1.017 455 000 000 000 0

Table 8: F/(CeO₂)₆, $\Delta E_{tot} = 1.49$ eV and $E_{ad} = -1.44$ eV.

F	1.940 636 000 000 000 0	0.414 418 000 000 000 0	-2.759 549 999 999 999 9
Ce	-0.121 597 000 000 000 0	-2.384 536 000 000 000 2	0.166 714 000 000 000 0
Ce	0.391 813 000 000 000 0	-0.048 128 000 000 000 0	2.771 875 999 999 999 8
Ce	-0.167 792 000 000 000 0	2.361 101 999 999 999 8	0.238 497 000 000 000 0
Ce	-2.742 166 000 000 000 1	-0.045 439 000 000 000 0	0.579 964 000 000 000 0
Ce	2.548 966 000 000 000 1	-0.051 103 000 000 000 0	-0.450 723 000 000 000 0
Ce	-0.439 908 000 000 000 0	-0.047 670 000 000 000 0	-2.550 141 000 000 000 0
O	1.419 179 000 000 000 0	-1.426 275 000 000 000 0	1.202 823 000 000 000 0
O	-1.216 483 000 000 000 0	1.477 784 999 999 999 9	1.733 991 000 000 000 1
O	0.769 489 000 000 000 0	-0.021 665 000 000 000 0	4.519 038 000 000 000 1
O	1.036 243 000 000 000 0	1.824 667 000 000 000 0	-1.486 756 000 000 000 0
O	-1.617 270 999 999 999 9	-1.424 096 000 000 000 0	-0.926 570 000 000 000 0
O	-1.199 784 000 000 000 0	-1.401 833 000 000 000 1	1.710 145 000 000 000 0
O	-1.538 002 000 000 000 1	1.356 053 000 000 000 0	-0.905 004 999 999 999 9
O	0.956 575 000 000 000 0	-1.549 746 000 000 000 1	-1.366 376 000 000 000 0
O	-4.513 185 000 000 000 0	-0.008 582 000 000 000 0	0.820 615 000 000 000 0
O	-1.195 634 000 000 000 1	-0.181 553 000 000 000 0	-4.154 964 999 999 999 8
O	4.312 379 000 000 000 0	-0.198 519 000 000 000 0	-0.278 075 000 000 000 0
O	1.376 538 000 000 000 0	1.355 113 000 000 000 0	1.134 498 999 999 999 9

Table 9: F/(CeO₂)₆, $\Delta E_{tot} = 0.69$ eV and $E_{ad} = -2.25$ eV.

F	3.853 515 999 999 999 9	1.309 088 000 000 000 0	-1.481 881 000 000 000 0
Ce	-0.010 923 000 000 000 0	-2.318 855 999 999 999 8	-0.081 285 000 000 000 0
Ce	0.316 770 000 000 000 0	-0.085 947 000 000 000 0	2.665 287 999 999 999 9
Ce	-0.383 050 000 000 000 0	2.323 592 000 000 000 1	0.121 458 000 000 000 0
Ce	-2.823 640 999 999 999 8	-0.229 779 000 000 000 0	0.522 877 000 000 000 0
Ce	2.406 718 000 000 000 1	0.234 785 000 000 000 0	-0.482 289 000 000 000 0
Ce	-0.716 695 000 000 000 0	0.087 417 000 000 000 0	-2.622 369 000 000 000 0
O	1.429 167 000 000 000 1	-1.322 195 000 000 000 0	1.012 386 000 000 000 0
O	-1.337 960 000 000 000 0	1.264 672 000 000 000 0	1.637 793 000 000 000 1
O	0.593 868 000 000 000 0	-0.128 488 000 000 000 0	4.428 949 000 000 000 2
O	0.717 060 000 000 000 0	1.556 197 000 000 000 1	-1.460 510 999 999 999 9
O	-1.624 549 999 999 999 9	-1.488 185 000 000 000 1	-1.107 898 000 000 000 0
O	-1.144 095 000 000 000 1	-1.564 541 000 000 000 0	1.509 073 000 000 000 1
O	-1.871 891 999 999 999 9	1.338 112 000 000 000 0	-0.968 331 000 000 000 1
O	0.992 651 000 000 000 0	-1.191 049 000 000 000 0	-1.577 529 000 000 000 0
O	-4.574 592 000 000 000 0	-0.371 264 000 000 000 0	0.848 396 000 000 000 0
O	-1.071 861 000 000 000 0	0.124 440 000 000 000 0	-4.373 019 000 000 000 2
O	3.971 248 000 000 000 1	-0.980 452 000 000 000 0	0.306 972 000 000 000 0
O	1.278 257 999 999 999 9	1.442 461 999 999 999 9	1.101 917 000 000 000 0

Table 10: F/(CeO₂)₆, $\Delta E_{tot} = 0.41$ eV and $E_{ad} = -2.53$ eV.

F	0.018 992 000 000 000 0	4.325 866 000 000 000 4	-0.313 432 000 000 000 0
Ce	0.071 774 000 000 000 0	-2.521 043 000 000 000 1	0.254 808 000 000 000 0
Ce	0.446 909 000 000 000 0	0.085 620 000 000 000 0	2.641 351 999 999 999 9
Ce	0.018 120 000 000 000 0	2.260 022 000 000 000 2	-0.165 861 000 000 000 0
Ce	-2.677 706 000 000 000 1	-0.287 602 000 000 000 0	0.567 205 000 000 000 0
Ce	2.636 130 999 999 999 8	-0.159 982 000 000 000 0	-0.449 057 000 000 000 0
Ce	-0.379 133 000 000 000 0	-0.552 154 000 000 000 0	-2.670 364 000 000 000 2
O	1.560 227 999 999 999 9	-1.453 060 000 000 000 0	1.222 947 999 999 999 9
O	-1.139 588 000 000 000 0	1.256 281 000 000 000 0	1.339 228 000 000 000 1
O	0.704 671 000 000 000 0	0.201 717 000 000 000 0	4.402 811 999 999 999 9
O	0.970 159 000 000 000 0	1.021 371 999 999 999 9	-1.636 665 000 000 000 0
O	-1.468 793 999 999 999 9	-1.664 253 999 999 999 9	-0.910 538 000 000 000 0
O	-1.064 746 000 000 000 0	-1.530 242 000 000 000 1	1.702 569 999 999 999 9
O	-1.796 913 999 999 999 9	1.013 431 000 000 000 0	-1.358 719 000 000 000 0
O	1.129 437 000 000 000 0	-1.774 172 000 000 000 1	-1.390 924 000 000 000 0
O	-4.403 113 000 000 000 3	-0.462 701 000 000 000 0	0.991 395 000 000 000 0
O	-0.545 216 000 000 000 0	-0.934 200 000 000 000 0	-4.405 802 000 000 000 4
O	4.384 933 000 000 000 2	-0.206 006 000 000 000 0	-0.799 677 000 000 000 0
O	1.533 863 000 000 000 0	1.381 105 999 999 999 9	0.978 716 999 999 999 9

Table 11: F/(CeO₂)₆, $\Delta E_{tot} = 0.00$ eV and $E_{ad} = -2.94$ eV.

F	-0.025 573 000 000 000 0	-4.321 457 999 999 999 8	-0.036 340 000 000 000 0
Ce	-0.015 182 000 000 000 0	-2.248 305 000 000 000 2	-0.018 380 000 000 000 0
Ce	0.448 653 000 000 000 0	0.189 376 000 000 000 0	2.470 723 000 000 000 0
Ce	0.003 245 000 000 000 0	2.553 834 000 000 000 2	-0.063 494 000 000 000 0
Ce	-2.647 791 999 999 999 9	0.211 008 000 000 000 0	0.474 324 000 000 000 0
Ce	2.646 681 000 000 000 1	0.177 980 000 000 000 0	-0.489 091 000 000 000 0
Ce	-0.479 681 000 000 000 0	0.148 048 000 000 000 0	-2.630 755 000 000 000 2
O	1.542 346 999 999 999 9	-1.126 630 000 000 000 0	1.175 603 000 000 000 0
O	-1.031 712 000 000 000 0	1.606 814 000 000 000 0	1.534 284 999 999 999 9
O	0.799 093 000 000 000 1	0.741 146 000 000 000 0	4.363 201 000 000 000 1
O	1.079 399 999 999 999 9	1.628 028 999 999 999 9	-1.554 846 000 000 000 0
O	-1.566 515 000 000 000 1	-1.199 206 000 000 000 0	-1.036 472 000 000 000 1
O	-1.042 639 000 000 000 1	-1.109 078 000 000 000 0	1.647 195 000 000 000 0
O	-1.538 678 999 999 999 9	1.644 385 000 000 000 0	-1.078 661 000 000 000 1
O	1.086 965 000 000 000 0	-1.215 505 000 000 000 1	-1.520 759 999 999 999 9
O	-4.392 662 999 999 999 8	0.299 825 000 000 000 0	0.837 633 000 000 000 0
O	-0.800 467 000 000 000 0	0.202 762 000 000 000 0	-4.385 563 000 000 000 3
O	4.410 522 000 000 000 3	0.226 497 000 000 000 0	-0.759 186 999 999 999 9
O	1.523 987 000 000 000 0	1.590 479 999 999 999 9	1.070 581 999 999 999 9

Table 12: Na/(CeO₂)₆, $\Delta E_{tot} = 0.74$ eV and $E_{ad} = -2.25$ eV.

Na	-6.105 249 999 999 999 8	-0.156 832 000 000 000 0	0.933 146 000 000 000 0
Ce	0.366 166 000 000 000 0	-2.453 091 999 999 999 8	-0.054 278 000 000 000 0
Ce	0.834 369 999 999 999 9	-0.018 976 000 000 000 0	2.566 644 999 999 999 8
Ce	0.384 585 000 000 000 0	2.365 091 000 000 000 1	-0.057 701 000 000 000 0
Ce	-2.153 277 999 999 999 8	-0.017 600 000 000 000 0	0.406 224 000 000 000 0
Ce	2.960 404 000 000 000 0	-0.031 143 000 000 000 0	-0.531 291 000 000 000 0
Ce	-0.125 484 000 000 000 0	-0.019 559 000 000 000 0	-2.669 430 000 000 000 2
O	1.937 200 000 000 000 0	-1.366 719 999 999 999 9	1.062 829 999 999 999 9
O	-0.732 505 000 000 000 0	1.442 652 000 000 000 0	1.488 728 000 000 000 1
O	1.065 409 000 000 000 1	-0.009 905 000 000 000 0	4.358 142 000 000 000 0
O	1.417 119 999 999 999 9	1.475 999 000 000 000 1	-1.604 168 000 000 000 0
O	-1.286 095 999 999 999 9	-1.349 979 000 000 000 0	-1.138 158 000 000 000 0
O	-0.794 436 999 999 999 9	-1.349 328 000 000 000 1	1.544 133 999 999 999 9
O	-1.208 547 000 000 000 0	1.441 227 000 000 000 0	-1.107 988 000 000 000 0
O	1.439 278 000 000 000 1	-1.368 025 000 000 000 0	-1.657 613 000 000 000 0
O	-4.082 969 000 000 000 3	-0.037 295 000 000 000 0	0.722 241 000 000 000 0
O	-0.548 114 000 000 000 0	-0.009 147 000 000 000 0	-4.426 287 999 999 999 6
O	4.734 029 999 999 999 7	-0.013 181 000 000 000 0	-0.856 100 000 000 000 0
O	1.898 109 000 000 000 0	1.475 808 999 999 999 9	1.020 917 000 000 000 1

Table 13: Na/(CeO₂)₆, $\Delta E_{tot} = 0.03$ eV and $E_{ad} = -2.96$ eV.

Na	-3.488 923 999 999 999 9	-1.027 287 000 000 000 1	-2.035 679 000 000 000 0
Ce	0.327 324 000 000 000 0	-2.369 092 999 999 999 9	0.316 844 000 000 000 0
Ce	0.889 491 000 000 000 0	0.242 588 000 000 000 0	2.722 062 999 999 999 9
Ce	0.232 848 000 000 000 0	2.443 588 000 000 000 1	0.015 194 000 000 000 0
Ce	-2.282 897 000 000 000 2	0.036 420 000 000 000 0	0.767 066 000 000 000 0
Ce	2.823 474 000 000 000 0	0.077 248 000 000 000 0	-0.515 100 000 000 000 0
Ce	-0.405 399 000 000 000 0	-0.122 384 000 000 000 0	-2.371 437 999 999 999 9
O	1.936 787 000 000 000 0	-1.176 166 000 000 000 0	1.220 153 000 000 000 0
O	-0.758 337 000 000 000 0	1.644 633 999 999 999 9	1.670 905 000 000 000 1
O	1.255 352 000 000 000 0	0.370 948 000 000 000 0	4.480 550 000 000 000 0
O	1.183 221 000 000 000 1	1.477 934 000 000 000 1	-1.576 935 000 000 000 0
O	-1.395 902 999 999 999 9	-1.390 878 000 000 000 1	-0.762 861 000 000 000 0
O	-0.760 738 000 000 000 0	-1.185 881 000 000 000 0	1.889 650 000 000 000 1
O	-1.361 113 000 000 000 0	1.360 305 000 000 000 1	-0.883 690 000 000 000 0
O	1.247 471 999 999 999 9	-1.358 328 000 000 000 0	-1.467 389 000 000 000 1
O	-3.990 426 999 999 999 9	-0.286 861 000 000 000 0	0.069 030 000 000 000 0
O	-1.839 042 000 000 000 1	-0.472 744 000 000 000 0	-3.524 067 000 000 000 1
O	4.549 223 999 999 999 7	0.090 141 000 000 000 0	-1.030 073 999 999 999 9
O	1.837 580 999 999 999 9	1.645 815 999 999 999 9	1.015 771 000 000 000 0

Table 14: Na/(CeO₂)₆, $\Delta E_{tot} = 0.03$ eV and $E_{ad} = -2.96$ eV.

Na	-3.091 775 000 000 000 2	1.215 167 000 000 000 1	-2.517 123 000 000 000 2
Ce	0.040 240 000 000 000 0	-2.454 902 999 999 999 8	0.101 912 000 000 000 0
Ce	0.493 078 000 000 000 0	-0.217 617 000 000 000 0	2.821 324 000 000 000 2
Ce	0.460 268 000 000 000 0	2.346 337 999 999 999 8	0.305 004 000 000 000 0
Ce	-2.363 607 000 000 000 0	0.152 785 000 000 000 0	0.447 022 000 000 000 0
Ce	2.854 991 000 000 000 1	-0.301 024 000 000 000 0	-0.120 212 000 000 000 0
Ce	-0.071 555 000 000 000 0	0.072 416 000 000 000 0	-2.405 323 999 999 999 8
O	1.552 337 000 000 000 1	-1.742 621 000 000 000 0	1.295 407 000 000 000 0
O	-0.915 784 000 000 000 0	1.297 962 000 000 000 1	1.738 610 000 000 000 0
O	0.612 143 000 000 000 0	-0.299 486 000 000 000 0	4.616 330 999 999 999 7
O	1.533 695 000 000 000 0	1.210 822 000 000 000 1	-1.312 117 000 000 000 0
O	-1.331 070 000 000 000 0	-1.286 574 000 000 000 1	-1.030 674 000 000 000 1
O	-1.101 955 999 999 999 9	-1.531 350 999 999 999 9	1.587 264 999 999 999 9
O	-1.169 586 999 999 999 9	1.461 810 000 000 000 1	-0.979 226 000 000 000 0
O	1.267 330 000 000 000 1	-1.615 920 999 999 999 9	-1.363 987 000 000 000 1
O	-3.930 295 000 000 000 1	0.582 373 000 000 000 0	-0.484 844 000 000 000 0
O	-1.305 960 999 999 999 9	0.489 018 000 000 000 0	-3.750 573 999 999 999 9
O	4.628 586 000 000 000 3	-0.449 210 000 000 000 0	-0.394 394 000 000 000 0
O	1.838 930 000 000 000 0	1.070 011 000 000 000 0	1.445 599 000 000 000 1

Table 15: Na/(CeO₂)₆, $\Delta E_{tot} = 0.03$ eV and $E_{ad} = -2.96$ eV.

Na	2.267 084 000 000 000 1	1.689 945 999 999 999 9	-3.059 870 999 999 999 8
Ce	0.251 858 000 000 000 0	-2.443 658 999 999 999 8	-0.047 787 000 000 000 0
Ce	0.198 441 000 000 000 0	-0.382 232 000 000 000 0	2.842 204 000 000 000 2
Ce	-0.625 984 000 000 000 0	2.260 034 999 999 999 8	0.553 071 000 000 000 0
Ce	-2.754 474 000 000 000 1	-0.638 580 000 000 000 0	0.503 497 000 000 000 0
Ce	2.374 741 000 000 000 2	0.416 788 000 000 000 0	-0.090 467 000 000 000 0
Ce	-0.493 750 000 000 000 0	0.170 903 000 000 000 0	-2.349 819 000 000 000 1
O	1.599 186 000 000 000 0	-1.448 361 999 999 999 9	1.196 550 999 999 999 9
O	-1.558 017 000 000 000 0	0.785 177 000 000 000 0	1.889 205 000 000 000 0
O	0.495 616 000 000 000 0	-0.557 443 000 000 000 0	4.609 691 999 999 999 9
O	0.749 202 000 000 000 0	1.628 304 999 999 999 9	-1.120 808 999 999 999 9
O	-1.365 216 999 999 999 9	-1.700 288 999 999 999 9	-1.144 339 999 999 999 9
O	-1.011 041 000 000 000 1	-1.963 022 000 000 000 0	1.497 369 000 000 000 0
O	-1.915 187 999 999 999 9	1.068 454 999 999 999 9	-0.851 552 000 000 000 0
O	1.189 181 000 000 000 0	-1.077 576 000 000 000 1	-1.384 450 000 000 000 0
O	-4.514 806 000 000 000 1	-1.000 688 999 999 999 9	0.617 725 000 000 000 0
O	0.337 480 000 000 000 0	0.794 946 000 000 000 0	-3.907 332 999 999 999 9
O	3.626 523 000 000 000 2	1.068 000 000 000 000 1	-1.321 125 000 000 000 1
O	1.149 162 000 000 000 0	1.329 298 000 000 000 1	1.568 233 999 999 999 9

Table 16: Na/(CeO₂)₆, $\Delta E_{tot} = 0.00$ eV and $E_{ad} = -2.99$ eV.

Na	-3.172 994 999 999 999 8	-1.014 996 000 000 000 0	-2.515 057 000 000 000 1
Ce	0.399 639 000 000 000 0	-2.374 544 000 000 000 2	0.217 762 000 000 000 0
Ce	0.541 301 000 000 000 0	0.102 738 000 000 000 0	2.822 436 000 000 000 2
Ce	0.114 258 000 000 000 0	2.443 814 999 999 999 8	0.188 097 000 000 000 0
Ce	-2.358 559 000 000 000 1	-0.106 179 000 000 000 0	0.479 714 000 000 000 0
Ce	2.862 890 999 999 999 9	0.221 557 000 000 000 0	-0.158 663 000 000 000 0
Ce	-0.108 507 000 000 000 0	0.009 081 000 000 000 0	-2.407 168 000 000 000 0
O	1.828 885 000 000 000 1	-1.170 508 000 000 000 1	1.376 730 999 999 999 9
O	-1.032 003 999 999 999 9	1.498 564 999 999 999 9	1.658 671 000 000 000 0
O	0.687 103 000 000 000 0	0.132 798 000 000 000 0	4.617 125 999 999 999 8
O	1.293 495 000 000 000 1	1.622 611 999 999 999 9	-1.326 341 999 999 999 9
O	-1.225 403 000 000 000 0	-1.395 108 999 999 999 9	-1.013 082 000 000 000 0
O	-0.924 497 000 000 000 0	-1.334 534 000 000 000 1	1.708 951 000 000 000 1
O	-1.304 605 000 000 000 0	1.354 518 000 000 000 1	-0.962 503 000 000 000 0
O	1.479 630 999 999 999 9	-1.208 253 000 000 000 0	-1.379 094 000 000 000 0
O	-3.955 363 999 999 999 9	-0.446 419 000 000 000 0	-0.438 178 000 000 000 0
O	-1.381 691 999 999 999 9	-0.306 563 000 000 000 0	-3.743 123 000 000 000 2
O	4.635 815 000 000 000 0	0.325 366 000 000 000 0	-0.456 479 000 000 000 0
O	1.620 613 000 000 000 1	1.646 055 000 000 000 0	1.330 203 000 000 000 0

Table 17: Ni/(CeO₂)₆, $\Delta E_{tot} = 1.50$ eV and $E_{ad} = -1.88$ eV.

Ni	-0.082 228 000 000 000 0	-0.499 538 000 000 000 0	-1.423 504 000 000 000 1
Ce	0.288 724 000 000 000 0	-2.362 740 000 000 000 1	0.631 003 000 000 000 0
Ce	0.484 173 000 000 000 0	0.476 905 000 000 000 0	2.742 935 000 000 000 1
Ce	-0.074 829 000 000 000 0	2.406 044 000 000 000 1	-0.180 906 000 000 000 0
Ce	-2.470 890 999 999 999 9	-0.117 263 000 000 000 0	0.435 339 000 000 000 0
Ce	2.667 300 000 000 000 0	0.007 698 000 000 000 0	-0.337 919 000 000 000 0
Ce	-1.035 534 000 000 000 0	1.011 193 000 000 000 0	-3.187 730 999 999 999 9
O	1.706 306 000 000 000 1	-1.058 885 000 000 000 1	1.540 813 000 000 000 0
O	-1.114 058 000 000 000 0	1.577 612 000 000 000 0	1.393 624 000 000 000 0
O	0.727 994 999 999 999 9	0.864 824 000 000 000 0	4.475 715 000 000 000 1
O	0.843 540 000 000 000 0	1.123 624 000 000 000 0	-1.784 621 000 000 000 0
O	-1.279 489 000 000 000 1	-1.711 260 999 999 999 9	-0.706 554 000 000 000 0
O	-0.943 714 000 000 000 1	-1.203 077 000 000 000 0	1.890 487 999 999 999 9
O	-1.765 358 999 999 999 9	1.914 187 000 000 000 1	-1.315 711 000 000 000 1
O	1.480 680 999 999 999 9	-1.855 328 000 000 000 1	-0.935 006 000 000 000 0
O	-4.231 461 000 000 000 4	-0.339 334 000 000 000 0	0.662 397 000 000 000 0
O	-1.062 157 999 999 999 9	2.253 603 000 000 000 0	-4.458 190 000 000 000 1
O	4.428 518 000 000 000 4	0.143 541 000 000 000 0	-0.614 097 000 000 000 0
O	1.519 535 000 000 000 1	1.705 166 000 000 000 0	0.897 049 000 000 000 0

Table 18: Ni/(CeO₂)₆, $\Delta E_{tot} = 1.16$ eV and $E_{ad} = -2.22$ eV.

Ni	2.070 361 000 000 000 1	1.268 316 000 000 000 0	-3.003 251 000 000 000 1
Ce	-0.139 123 000 000 000 0	-2.391 312 000 000 000 1	0.199 365 000 000 000 0
Ce	0.360 487 000 000 000 0	-0.020 207 000 000 000 0	2.794 805 000 000 000 2
Ce	-0.080 943 000 000 000 0	2.290 252 000 000 000 2	0.130 869 000 000 000 0
Ce	-2.745 232 000 000 000 1	-0.015 319 000 000 000 0	0.607 920 000 000 000 0
Ce	2.579 753 999 999 999 9	-0.139 244 000 000 000 0	-0.311 556 000 000 000 0
Ce	-0.582 018 000 000 000 0	-0.136 579 000 000 000 0	-2.530 927 999 999 999 8
O	1.411 392 999 999 999 9	-1.487 984 000 000 000 0	1.262 658 000 000 000 1
O	-1.168 582 999 999 999 9	1.428 213 000 000 000 0	1.672 377 000 000 000 0
O	0.656 623 000 000 000 0	0.036 478 000 000 000 0	4.558 531 000 000 000 3
O	1.063 183 999 999 999 9	1.480 471 000 000 000 1	-1.486 752 000 000 000 1
O	-1.664 249 000 000 000 1	-1.485 570 000 000 000 1	-0.897 346 000 000 000 0
O	-1.209 460 000 000 000 0	-1.410 812 000 000 000 0	1.724 023 000 000 000 1
O	-1.580 602 000 000 000 1	1.333 091 999 999 999 9	-0.951 070 000 000 000 0
O	0.949 562 000 000 000 0	-1.500 925 000 000 000 1	-1.348 856 000 000 000 1
O	-4.507 884 999 999 999 9	0.043 886 000 000 000 0	0.909 143 000 000 000 0
O	-1.210 673 000 000 000 1	-0.308 472 000 000 000 0	-4.193 448 000 000 000 1
O	4.357 203 000 000 000 2	-0.313 010 000 000 000 0	-0.313 361 000 000 000 0
O	1.440 196 000 000 000 0	1.328 721 000 000 000 0	1.176 879 000 000 000 0

Table 19: Ni/(CeO₂)₆, $\Delta E_{tot} = 0.73$ eV and $E_{ad} = -2.65$ eV.

Ni	-2.006 971 000 000 000 1	-3.045 675 999 999 999 8	-1.357 790 000 000 000 1
Ce	0.240 777 000 000 000 0	-2.245 890 999 999 999 9	0.176 544 000 000 000 0
Ce	0.595 287 000 000 000 0	0.228 992 000 000 000 0	2.711 552 000 000 000 2
Ce	0.075 600 000 000 000 0	2.508 778 000 000 000 0	0.038 209 000 000 000 0
Ce	-2.522 111 999 999 999 9	0.137 982 000 000 000 0	0.584 276 000 000 000 0
Ce	2.744 635 999 999 999 9	0.211 712 000 000 000 0	-0.421 920 000 000 000 0
Ce	-0.361 710 000 000 000 0	0.121 208 000 000 000 0	-2.565 064 000 000 000 0
O	1.735 624 000 000 000 1	-1.220 420 000 000 000 1	1.197 551 999 999 999 9
O	-0.979 489 000 000 000 1	1.624 668 000 000 000 0	1.611 086 000 000 000 0
O	0.889 400 000 000 000 0	0.261 101 000 000 000 0	4.478 907 999 999 999 7
O	1.159 144 000 000 000 0	1.607 747 000 000 000 0	-1.505 162 000 000 000 1
O	-1.559 601 000 000 000 0	-1.298 163 000 000 000 0	-1.065 223 999 999 999 9
O	-0.920 651 000 000 000 0	-1.204 051 000 000 000 0	1.631 613 999 999 999 9
O	-1.450 177 000 000 000 0	1.519 763 000 000 000 0	-1.003 468 999 999 999 9
O	1.186 016 000 000 000 0	-1.221 062 000 000 000 1	-1.437 619 000 000 000 0
O	-4.285 549 999 999 999 7	0.089 215 000 000 000 0	0.909 549 000 000 000 1
O	-0.681 152 000 000 000 0	0.062 544 000 000 000 0	-4.329 261 999 999 999 9
O	4.502 417 999 999 999 6	0.231 880 000 000 000 0	-0.769 760 000 000 000 0
O	1.638 504 000 000 000 0	1.629 675 000 000 000 0	1.115 980 999 999 999 9

Table 20: Ni/(CeO₂)₆, $\Delta E_{tot} = 0.58$ eV and $E_{ad} = -2.80$ eV.

Ni	-2.781 232 000 000 000 1	1.249 144 999 999 999 9	-0.875 799 000 000 000 0
Ce	0.412 896 000 000 000 0	-2.472 499 000 000 000 0	0.117 458 000 000 000 0
Ce	0.726 237 000 000 000 0	-0.053 423 000 000 000 0	2.706 598 000 000 000 1
Ce	-0.080 860 000 000 000 0	2.255 990 999 999 999 9	0.035 697 000 000 000 0
Ce	-2.471 785 000 000 000 1	-0.626 147 000 000 000 0	0.916 520 000 000 000 0
Ce	2.760 018 000 000 000 1	0.108 185 000 000 000 0	-0.447 912 000 000 000 0
Ce	-0.566 633 000 000 000 1	-0.080 507 000 000 000 0	-2.462 075 000 000 000 0
O	1.878 101 999 999 999 9	-1.378 547 000 000 000 0	1.144 671 000 000 000 0
O	-1.037 805 000 000 000 1	0.947 883 999 999 999 9	1.548 748 000 000 000 0
O	0.914 091 000 000 000 0	0.104 197 000 000 000 0	4.484 093 999 999 999 8
O	1.063 712 999 999 999 9	1.230 506 000 000 000 1	-1.436 612 999 999 999 9
O	-1.338 028 999 999 999 9	-1.583 814 000 000 000 1	-0.741 020 000 000 000 0
O	-0.697 506 000 000 000 0	-1.810 263 000 000 000 0	1.809 758 999 999 999 9
O	-1.377 075 000 000 000 0	2.113 617 000 000 000 1	-1.541 828 000 000 000 0
O	1.237 093 000 000 000 0	-1.518 285 000 000 000 1	-1.443 403 000 000 000 0
O	-3.967 106 999 999 999 9	0.218 505 000 000 000 0	0.063 462 000 000 000 0
O	-0.750 540 000 000 000 0	-0.414 662 000 000 000 0	-4.203 217 999 999 999 7
O	4.510 720 000 000 000 1	0.222 877 000 000 000 0	-0.815 650 000 000 000 0
O	1.565 693 000 000 000 0	1.487 247 999 999 999 9	1.140 511 000 000 000 1

Table 21: Ni/(CeO₂)₆, $\Delta E_{tot} = 0.00$ eV and $E_{ad} = -3.38$ eV.

Ni	-5.885 194 000 000 000 3	-0.174 235 000 000 000 0	0.911 793 000 000 000 0
Ce	0.352 233 000 000 000 0	-2.457 545 000 000 000 1	-0.052 164 000 000 000 0
Ce	0.827 818 000 000 000 1	-0.019 434 000 000 000 0	2.575 606 000 000 000 1
Ce	0.384 021 000 000 000 0	2.370 544 999 999 999 9	-0.058 566 000 000 000 0
Ce	-2.138 463 999 999 999 9	-0.008 617 000 000 000 0	0.400 655 000 000 000 0
Ce	2.954 346 999 999 999 8	-0.035 026 000 000 000 0	-0.529 887 000 000 000 0
Ce	-0.132 588 000 000 000 0	-0.018 445 000 000 000 0	-2.678 621 999 999 999 8
O	1.914 889 000 000 000 1	-1.364 416 000 000 000 1	1.061 738 000 000 000 1
O	-0.753 548 000 000 000 0	1.424 322 000 000 000 1	1.477 854 999 999 999 9
O	1.091 904 999 999 999 9	-0.011 587 000 000 000 0	4.354 700 000 000 000 2
O	1.403 152 000 000 000 0	1.478 498 000 000 000 1	-1.600 394 000 000 000 1
O	-1.313 512 999 999 999 9	-1.326 854 999 999 999 9	-1.114 972 000 000 000 1
O	-0.827 321 000 000 000 0	-1.328 198 999 999 999 9	1.529 930 000 000 000 0
O	-1.219 300 000 000 000 1	1.424 369 999 999 999 9	-1.095 750 000 000 000 0
O	1.418 393 999 999 999 9	-1.364 703 999 999 999 9	-1.648 335 000 000 000 1
O	-4.163 948 999 999 999 7	-0.038 780 000 000 000 0	0.732 643 000 000 000 0
O	-0.516 267 000 000 000 0	-0.010 954 000 000 000 0	-4.436 060 999 999 999 6
O	4.722 603 000 000 000 3	-0.017 081 000 000 000 0	-0.853 709 000 000 000 1
O	1.880 775 000 000 000 1	1.478 138 000 000 000 0	1.023 530 000 000 000 1

Table 22: Pd/(CeO₂)₆, $\Delta E_{tot} = 0.56$ eV and $E_{ad} = -0.65$ eV.

Pd	1.344 484 000 000 000 0	0.197 275 000 000 000 0	-1.959 111 000 000 000 0
Ce	0.150 289 000 000 000 0	-1.976 326 999 999 999 9	-0.073 105 000 000 000 0
Ce	0.446 379 000 000 000 0	0.304 447 000 000 000 0	2.664 067 999 999 999 9
Ce	0.031 465 000 000 000 0	2.424 843 000 000 000 1	-0.206 763 000 000 000 0
Ce	-2.657 083 999 999 999 8	0.185 556 000 000 000 0	0.529 814 000 000 000 0
Ce	3.149 601 999 999 999 8	-0.176 525 000 000 000 0	0.227 878 000 000 000 0
Ce	-1.340 027 000 000 000 1	0.604 093 000 000 000 0	-2.873 683 999 999 999 9
O	1.634 919 000 000 000 0	-1.248 076 000 000 000 0	1.401 928 000 000 000 1
O	-1.005 322 000 000 000 0	1.647 030 000 000 000 0	1.448 110 000 000 000 0
O	0.649 185 000 000 000 0	0.497 428 000 000 000 0	4.431 006 000 000 000 0
O	0.519 529 000 000 000 0	2.051 251 000 000 000 2	-2.164 460 000 000 000 1
O	-1.430 582 999 999 999 9	-1.048 556 000 000 000 0	-1.189 383 000 000 000 1
O	-1.014 715 000 000 000 0	-1.157 554 000 000 000 0	1.475 009 000 000 000 0
O	-1.885 111 000 000 000 0	1.705 284 000 000 000 0	-1.054 926 000 000 000 0
O	1.811 882 999 999 999 9	-1.648 552 000 000 000 0	-1.233 649 000 000 000 0
O	-4.385 000 999 999 999 9	0.016 347 000 000 000 0	0.961 672 000 000 000 0
O	-2.416 027 999 999 999 8	0.683 638 000 000 000 0	-4.293 292 000 000 000 1
O	4.854 086 999 999 999 8	-0.225 268 000 000 000 0	0.749 021 000 000 000 0
O	1.629 092 999 999 999 9	1.500 637 999 999 999 9	0.884 992 000 000 000 0

Table 23: Pd/(CeO₂)₆, $\Delta E_{tot} = 0.25$ eV and $E_{ad} = -0.95$ eV.

Pd	-5.123 413 000 000 000 2	-0.855 884 000 000 000 0	0.011 633 000 000 000 0
Ce	0.189 763 000 000 000 0	-2.297 712 999 999 999 9	-0.001 229 000 000 000 0
Ce	0.844 971 999 999 999 9	0.030 320 000 000 000 0	2.613 027 999 999 999 9
Ce	0.376 479 000 000 000 0	2.366 524 000 000 000 1	-0.030 312 000 000 000 0
Ce	-2.323 248 000 000 000 0	0.144 395 000 000 000 0	0.547 105 000 000 000 0
Ce	2.903 497 000 000 000 2	-0.071 531 000 000 000 0	-0.576 361 000 000 000 0
Ce	-0.285 385 000 000 000 0	0.035 656 000 000 000 0	-2.641 538 000 000 000 2
O	1.801 115 000 000 000 0	-1.438 987 000 000 000 0	1.018 353 000 000 000 1
O	-0.676 730 000 000 000 1	1.497 848 000 000 000 1	1.550 041 000 000 000 0
O	1.205 330 999 999 999 9	0.017 377 000 000 000 0	4.365 378 999 999 999 9
O	1.354 743 999 999 999 9	1.399 709 000 000 000 1	-1.604 165 000 000 000 1
O	-1.346 025 000 000 000 0	-1.323 172 000 000 000 0	-1.026 527 000 000 000 0
O	-0.799 868 000 000 000 0	-1.314 991 000 000 000 0	1.569 031 000 000 000 1
O	-1.245 377 000 000 000 0	1.496 490 000 000 000 1	-1.039 743 000 000 000 1
O	1.248 005 000 000 000 0	-1.433 646 000 000 000 0	-1.585 283 999 999 999 9
O	-4.060 889 999 999 999 7	0.455 858 000 000 000 0	1.160 738 000 000 000 0
O	-0.637 843 000 000 000 0	0.029 255 000 000 000 0	-4.395 780 000 000 000 2
O	4.656 083 999 999 999 9	-0.132 287 000 000 000 0	-0.932 072 000 000 000 0
O	1.918 786 000 000 000 1	1.394 768 000 000 000 0	0.997 691 000 000 000 0

Table 24: Pd/(CeO₂)₆, $\Delta E_{tot} = 0.19$ eV and $E_{ad} = -1.01$ eV.

Pd	2.238 839 000 000 000 0	1.219 632 000 000 000 0	-3.088 001 999 999 999 9
Ce	-0.157 545 000 000 000 0	-2.385 672 000 000 000 0	0.214 520 000 000 000 0
Ce	0.356 913 000 000 000 0	-0.004 018 000 000 000 0	2.800 284 000 000 000 0
Ce	-0.092 745 000 000 000 0	2.288 393 000 000 000 1	0.123 937 000 000 000 0
Ce	-2.759 770 000 000 000 1	-0.004 249 000 000 000 0	0.622 920 999 999 999 9
Ce	2.560 655 999 999 999 8	-0.138 361 000 000 000 0	-0.309 737 000 000 000 0
Ce	-0.589 188 000 000 000 0	-0.131 475 000 000 000 0	-2.512 840 000 000 000 2
O	1.395 141 000 000 000 0	-1.481 236 000 000 000 0	1.273 937 000 000 000 1
O	-1.176 536 999 999 999 9	1.438 636 999 999 999 9	1.675 130 000 000 000 0
O	0.675 810 000 000 000 0	0.060 974 000 000 000 0	4.560 170 000 000 000 3
O	1.010 181 999 999 999 9	1.410 417 999 999 999 9	-1.467 668 999 999 999 9
O	-1.683 808 999 999 999 9	-1.478 070 000 000 000 0	-0.882 337 000 000 000 0
O	-1.223 078 000 000 000 1	-1.399 534 000 000 000 1	1.739 525 000 000 000 0
O	-1.611 183 000 000 000 0	1.342 984 000 000 000 0	-0.947 091 000 000 000 0
O	0.932 370 999 999 999 9	-1.519 004 000 000 000 0	-1.340 635 000 000 000 0
O	-4.522 280 000 000 000 3	0.056 685 000 000 000 0	0.928 430 000 000 000 0
O	-1.126 854 999 999 999 9	-0.289 314 000 000 000 0	-4.210 473 999 999 999 6
O	4.337 436 000 000 000 3	-0.327 754 000 000 000 0	-0.358 713 000 000 000 0
O	1.435 639 000 000 000 1	1.340 958 000 000 000 1	1.178 644 999 999 999 9

Table 25: Pd/(CeO₂)₆, $\Delta E_{tot} = 0.06$ eV and $E_{ad} = -1.14$ eV.

Pd	-2.682 834 000 000 000 2	1.469 486 000 000 000 1	-1.056 943 000 000 000 0
Ce	0.448 510 000 000 000 0	-2.537 361 999 999 999 9	0.223 609 000 000 000 0
Ce	0.735 155 000 000 000 0	-0.009 290 000 000 000 0	2.712 543 000 000 000 1
Ce	-0.095 713 000 000 000 0	2.374 042 000 000 000 2	0.095 965 000 000 000 0
Ce	-2.434 205 000 000 000 0	-0.638 035 000 000 000 0	0.905 792 000 000 000 0
Ce	2.660 407 000 000 000 2	0.124 406 000 000 000 0	-0.493 103 000 000 000 0
Ce	-0.541 990 000 000 000 0	-0.370 737 000 000 000 0	-2.470 072 000 000 000 0
O	1.883 914 000 000 000 1	-1.391 030 999 999 999 9	1.168 712 999 999 999 9
O	-1.061 415 000 000 000 0	0.931 908 000 000 000 0	1.576 554 999 999 999 9
O	0.947 433 000 000 000 0	0.167 795 000 000 000 0	4.484 874 999 999 999 7
O	0.813 132 000 000 000 0	1.119 991 000 000 000 0	-1.453 541 999 999 999 9
O	-1.307 444 000 000 000 1	-1.693 378 000 000 000 0	-0.680 273 000 000 000 0
O	-0.695 629 000 000 000 1	-1.810 586 999 999 999 9	1.861 266 000 000 000 1
O	-1.390 245 000 000 000 0	3.040 213 000 000 000 1	-1.135 783 999 999 999 9
O	1.232 494 000 000 000 0	-1.630 443 000 000 000 1	-1.413 794 999 999 999 9
O	-3.787 547 000 000 000 0	-0.083 902 000 000 000 0	-0.295 045 000 000 000 0
O	-0.701 296 000 000 000 0	-0.853 512 000 000 000 0	-4.177 829 000 000 000 0
O	4.373 348 000 000 000 0	0.317 455 000 000 000 0	-0.978 580 000 000 000 0
O	1.603 925 000 000 000 0	1.472 976 000 000 000 1	1.125 647 000 000 000 1

Table 26: Pd/(CeO₂)₆, $\Delta E_{tot} = 0.00$ eV and $E_{ad} = -1.20$ eV.

Pd	-1.988 634 999 999 999 9	-3.273 229 999 999 999 9	-1.261 810 000 000 000 1
Ce	0.204 781 000 000 000 0	-2.199 371 999 999 999 9	0.145 261 000 000 000 0
Ce	0.604 906 000 000 000 1	0.230 709 000 000 000 0	2.712 689 000 000 000 1
Ce	0.068 483 000 000 000 0	2.504 267 000 000 000 0	0.034 145 000 000 000 0
Ce	-2.537 364 999 999 999 9	0.136 388 000 000 000 0	0.559 102 000 000 000 0
Ce	2.752 794 999 999 999 9	0.218 576 000 000 000 0	-0.415 694 000 000 000 0
Ce	-0.381 017 000 000 000 0	0.127 078 000 000 000 0	-2.577 000 000 000 000 0
O	1.724 105 000 000 000 0	-1.218 629 000 000 000 0	1.184 550 000 000 000 0
O	-0.976 662 000 000 000 0	1.606 138 000 000 000 1	1.599 436 000 000 000 1
O	0.890 821 000 000 000 0	0.245 944 000 000 000 0	4.479 576 999 999 999 9
O	1.152 849 999 999 999 9	1.593 822 000 000 000 1	-1.498 844 000 000 000 1
O	-1.515 571 999 999 999 9	-1.272 987 000 000 000 1	-1.042 851 000 000 000 0
O	-0.905 511 000 000 000 0	-1.214 010 000 000 000 0	1.617 291 000 000 000 0
O	-1.461 030 000 000 000 1	1.529 941 999 999 999 9	-1.014 831 000 000 000 0
O	1.183 829 999 999 999 9	-1.227 582 000 000 000 0	-1.427 065 999 999 999 9
O	-4.294 927 999 999 999 6	0.181 892 000 000 000 0	0.895 112 000 000 000 0
O	-0.672 087 000 000 000 0	0.171 573 000 000 000 0	-4.342 506 000 000 000 2
O	4.508 365 000 000 000 4	0.231 645 000 000 000 0	-0.764 575 000 000 000 0
O	1.641 867 000 000 000 0	1.627 837 999 999 999 9	1.118 020 999 999 999 9

Table 27: Pt/(CeO₂)₆, $\Delta E_{tot} = 2.36$ eV and $E_{ad} = -0.93$ eV.

Pt	-0.168 976 000 000 000 0	-4.938 510 000 000 000 0	1.291 743 000 000 000 1
Ce	0.024 725 000 000 000 0	-2.062 374 999 999 999 8	-0.126 155 000 000 000 0
Ce	0.492 624 000 000 000 0	0.218 784 000 000 000 0	2.563 206 999 999 999 8
Ce	-0.003 268 000 000 000 0	2.610 777 000 000 000 1	-0.023 598 000 000 000 0
Ce	-2.628 185 000 000 000 2	0.249 142 000 000 000 0	0.413 406 000 000 000 0
Ce	2.649 541 000 000 000 1	0.301 403 000 000 000 0	-0.557 114 000 000 000 0
Ce	-0.475 677 000 000 000 0	0.330 514 000 000 000 0	-2.711 797 999 999 999 9
O	1.570 762 000 000 000 0	-1.144 172 000 000 000 0	0.966 585 000 000 000 0
O	-1.067 689 000 000 000 1	1.655 125 000 000 000 0	1.507 311 000 000 000 1
O	0.803 675 000 000 000 0	0.146 476 000 000 000 0	4.327 350 000 000 000 0
O	1.070 927 000 000 000 0	1.737 080 000 000 000 0	-1.592 713 000 000 000 0
O	-1.536 586 000 000 000 0	-1.117 351 999 999 999 9	-1.175 546 000 000 000 0
O	-1.055 118 999 999 999 9	-1.179 692 000 000 000 0	1.452 512 000 000 000 0
O	-1.548 035 000 000 000 0	1.713 641 000 000 000 0	-1.110 932 000 000 000 0
O	1.093 399 999 999 999 9	-1.096 710 000 000 000 1	-1.662 177 999 999 999 9
O	-4.389 268 999 999 999 6	0.222 312 000 000 000 0	0.744 197 000 000 000 0
O	-0.799 665 000 000 000 0	0.361 135 000 000 000 0	-4.473 715 999 999 999 6
O	4.415 769 000 000 000 1	0.306 657 000 000 000 0	-0.858 851 999 999 999 9
O	1.551 047 000 000 000 1	1.685 766 000 000 000 1	1.026 286 000 000 000 0

Table 28: Pt/(CeO₂)₆, $\Delta E_{tot} = 0.90$ eV and $E_{ad} = -2.39$ eV.

Pt	2.167 587 000 000 000 2	1.224 232 000 000 000 0	-3.078 114 999 999 999 9
Ce	-0.142 684 000 000 000 0	-2.381 246 000 000 000 0	0.196 713 000 000 000 0
Ce	0.362 074 000 000 000 0	-0.020 110 000 000 000 0	2.789 689 999 999 999 8
Ce	-0.093 743 000 000 000 0	2.300 399 999 999 999 8	0.137 532 000 000 000 0
Ce	-2.748 845 999 999 999 9	-0.015 985 000 000 000 0	0.606 597 000 000 000 1
Ce	2.596 086 999 999 999 8	-0.136 550 000 000 000 0	-0.330 792 000 000 000 0
Ce	-0.568 344 000 000 000 0	-0.131 447 000 000 000 0	-2.550 492 999 999 999 9
O	1.402 323 999 999 999 9	-1.478 436 000 000 000 1	1.258 305 000 000 000 0
O	-1.174 086 000 000 000 0	1.451 065 000 000 000 0	1.674 312 999 999 999 9
O	0.664 230 000 000 000 0	0.036 047 000 000 000 0	4.551 568 999 999 999 8
O	1.071 202 999 999 999 9	1.530 423 000 000 000 1	-1.524 725 000 000 000 1
O	-1.664 579 000 000 000 0	-1.473 660 000 000 000 0	-0.894 782 000 000 000 0
O	-1.216 755 999 999 999 9	-1.393 894 000 000 000 0	1.728 720 000 000 000 0
O	-1.566 711 000 000 000 0	1.337 620 000 000 000 0	-0.948 214 000 000 000 0
O	0.944 634 000 000 000 0	-1.496 902 000 000 000 0	-1.347 491 999 999 999 9
O	-4.509 155 999 999 999 9	0.044 059 000 000 000 0	0.917 674 000 000 000 0
O	-1.307 456 000 000 000 0	-0.354 194 000 000 000 0	-4.158 228 000 000 000 3
O	4.356 863 999 999 999 8	-0.373 830 000 000 000 0	-0.179 955 000 000 000 0
O	1.427 357 999 999 999 9	1.332 406 999 999 999 9	1.151 683 999 999 999 9

Table 29: Pt/(CeO₂)₆, $\Delta E_{tot} = 0.60$ eV and $E_{ad} = -2.68$ eV.

Pt	-1.554 958 000 000 000 1	-3.032 220 000 000 000 1	2.022 956 999 999 999 9
Ce	0.036 167 000 000 000 0	-2.254 049 000 000 000 2	-0.119 204 000 000 000 0
Ce	0.602 865 000 000 000 0	0.210 385 000 000 000 0	2.550 346 999 999 999 9
Ce	0.167 555 000 000 000 0	2.471 611 999 999 999 9	-0.165 527 000 000 000 0
Ce	-2.584 870 000 000 000 0	0.275 825 000 000 000 0	0.361 419 000 000 000 0
Ce	2.719 774 999 999 999 8	0.040 339 000 000 000 0	-0.606 448 000 000 000 0
Ce	-0.399 381 000 000 000 0	0.105 291 000 000 000 0	-2.753 063 000 000 000 0
O	1.530 736 000 000 000 1	-1.262 180 000 000 000 1	0.965 803 000 000 000 0
O	-0.923 162 000 000 000 0	1.586 778 999 999 999 9	1.396 095 000 000 000 1
O	1.042 683 000 000 000 0	0.407 365 000 000 000 0	4.270 483 999 999 999 7
O	1.201 989 000 000 000 0	1.471 692 000 000 000 0	-1.697 767 000 000 000 0
O	-1.476 245 999 999 999 9	-1.193 665 000 000 000 0	-1.108 171 000 000 000 0
O	-1.155 554 000 000 000 0	-1.170 933 000 000 000 0	1.651 206 000 000 000 0
O	-1.414 156 000 000 000 0	1.615 587 000 000 000 1	-1.213 819 000 000 000 0
O	1.124 760 999 999 999 9	-1.383 464 000 000 000 0	-1.672 385 000 000 000 0
O	-4.336 450 000 000 000 1	0.528 238 000 000 000 0	0.605 496 000 000 000 0
O	-0.752 566 000 000 000 0	0.058 558 000 000 000 0	-4.505 981 000 000 000 2
O	4.482 848 999 999 999 9	-0.021 559 000 000 000 0	-0.901 354 000 000 000 0
O	1.687 963 000 000 000 1	1.546 403 000 000 000 0	0.919 918 000 000 000 0

Table 30: Pt/(CeO₂)₆, $\Delta E_{tot} = 0.48$ eV and $E_{ad} = -2.80$ eV.

Pt	1.290 499 000 000 000 1	0.202 481 000 000 000 0	-1.869 151 999 999 999 9
Ce	0.031 760 000 000 000 0	-1.926 350 999 999 999 9	-0.198 755 000 000 000 0
Ce	0.449 248 000 000 000 0	0.176 971 000 000 000 0	2.664 054 999 999 999 8
Ce	0.190 635 000 000 000 0	2.377 216 999 999 999 9	-0.139 147 000 000 000 0
Ce	-2.660 177 000 000 000 0	0.313 299 000 000 000 0	0.514 073 000 000 000 0
Ce	3.201 687 000 000 000 2	0.566 685 000 000 000 0	0.268 464 000 000 000 0
Ce	-1.393 988 999 999 999 9	-0.140 566 000 000 000 0	-2.897 809 000 000 000 1
O	1.637 912 000 000 000 0	-1.089 237 000 000 000 0	0.947 317 000 000 000 0
O	-0.982 288 000 000 000 0	1.636 649 999 999 999 9	1.426 911 000 000 000 0
O	0.610 622 000 000 000 0	0.056 007 000 000 000 0	4.440 882 000 000 000 2
O	1.931 702 999 999 999 9	2.007 782 000 000 000 2	-1.283 828 000 000 000 0
O	-1.890 967 000 000 000 1	-1.227 695 000 000 000 0	-1.053 452 000 000 000 1
O	-1.012 655 000 000 000 1	-1.150 755 000 000 000 0	1.439 789 999 999 999 9
O	-1.457 430 000 000 000 0	1.541 485 999 999 999 9	-1.224 275 000 000 000 0
O	0.493 202 000 000 000 0	-1.597 615 999 999 999 9	-2.236 193 999 999 999 8
O	-4.375 897 000 000 000 1	0.472 728 000 000 000 0	0.991 649 000 000 000 0
O	-2.526 686 999 999 999 9	-0.189 521 000 000 000 0	-4.273 601 000 000 000 2
O	4.888 899 999 999 999 6	0.622 049 000 000 000 0	0.841 539 000 000 000 0
O	1.660 974 000 000 000 0	1.685 354 000 000 000 0	1.366 657 000 000 000 0

Table 31: Pt/(CeO₂)₆, $\Delta E_{tot} = 0.00$ eV and $E_{ad} = -3.28$ eV

Pt	-2.624 343 000 000 000 1	1.449 731 000 000 000 1	-1.008 016 999 999 999 9
Ce	0.451 011 000 000 000 0	-2.539 031 000 000 000 0	0.227 065 000 000 000 0
Ce	0.743 368 000 000 000 0	-0.016 719 000 000 000 0	2.723 940 999 999 999 9
Ce	-0.109 928 000 000 000 0	2.352 078 999 999 999 8	0.093 466 000 000 000 0
Ce	-2.418 499 999 999 999 9	-0.616 589 000 000 000 1	0.892 353 000 000 000 0
Ce	2.656 216 000 000 000 1	0.123 938 000 000 000 0	-0.495 282 000 000 000 0
Ce	-0.566 857 000 000 000 1	-0.363 791 000 000 000 0	-2.468 249 000 000 000 1
O	1.888 705 000 000 000 1	-1.391 761 000 000 000 0	1.170 026 000 000 000 0
O	-1.051 557 000 000 000 1	0.931 356 000 000 000 0	1.619 323 000 000 000 1
O	0.964 474 000 000 000 1	0.155 637 000 000 000 0	4.495 620 999 999 999 9
O	0.809 122 000 000 000 0	1.131 084 999 999 999 9	-1.449 654 999 999 999 9
O	-1.313 825 000 000 000 0	-1.704 923 000 000 000 0	-0.672 986 000 000 000 0
O	-0.691 774 000 000 000 0	-1.802 114 999 999 999 9	1.859 761 999 999 999 9
O	-1.425 291 000 000 000 1	3.036 652 999 999 999 8	-1.187 488 000 000 000 1
O	1.224 493 000 000 000 1	-1.625 132 999 999 999 9	-1.407 276 999 999 999 9
O	-3.788 717 999 999 999 8	-0.063 688 000 000 000 0	-0.365 372 000 000 000 0
O	-0.710 403 000 000 000 0	-0.851 543 000 000 000 0	-4.175 921 999 999 999 9
O	4.371 108 999 999 999 7	0.320 891 000 000 000 0	-0.971 588 000 000 000 0
O	1.592 697 999 999 999 9	1.473 919 999 999 999 9	1.120 277 000 000 000 0