Modulation of Superficial Electronic Structure via Metal-Support Interaction for H_2 Evolution over Pd Catalysts

Jin Wang,[a] Dan Cheng,[b,c] Mengmeng Gao,[a] Qian Li,[a] Ying Xin,[a] Nana Zhang,[a] Zhaoliang Zhang,*[a,d] Xuehua Yu,[d] Zhen Zhao,*[d] and Kebin Zhou,*[b]

a School of Chemistry and Chemical Engineering, Shandong Provincial Key Laboratory of Fluorine Chemistry and Chemical Materials, University of Jinan, Jinan 250022, P.R. China.Email: chm_zhangzl@ujn.edu.cn

b School of Chemical Sciences, University of Chinese Academy of Sciences, Beijing 100049, P.R. China. Email: kbzhou@ucas.ac.cn

c Department of Biological Sciences, National University of Singapore, 117543, Singapore.

d Institute of Catalysis for Energy and Environment, College of Chemistry and Chemical Engineering, Shenyang Normal University, Shenyang 110034, Liaoning, P. R. China. Email: zhenzhao@cup.edu.cn

1. Supplementary Results

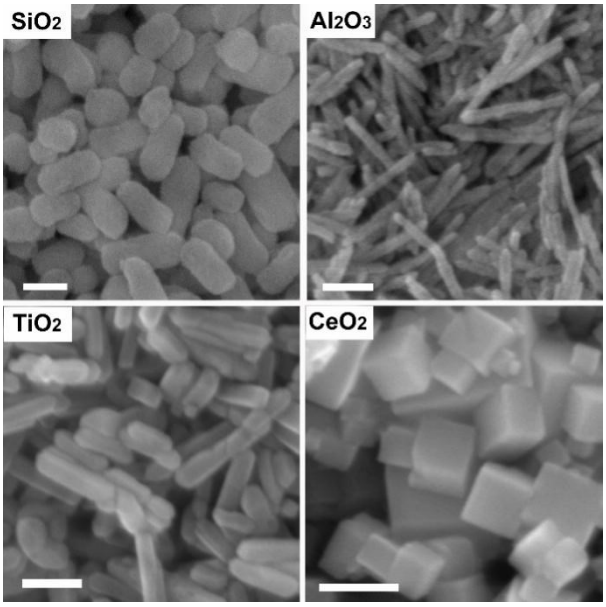

Figure S1. SEM images of the four metal oxide supports: SiO_2, Al_2O_3, TiO_2 and CeO_2.

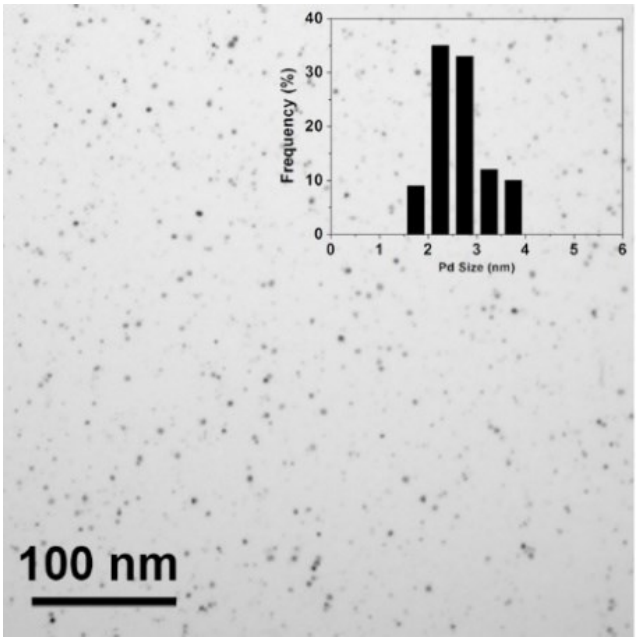

Figure S2. TEM images of colloidal Pd nanoparticles and the histogram of the particle-size distributions (inset).

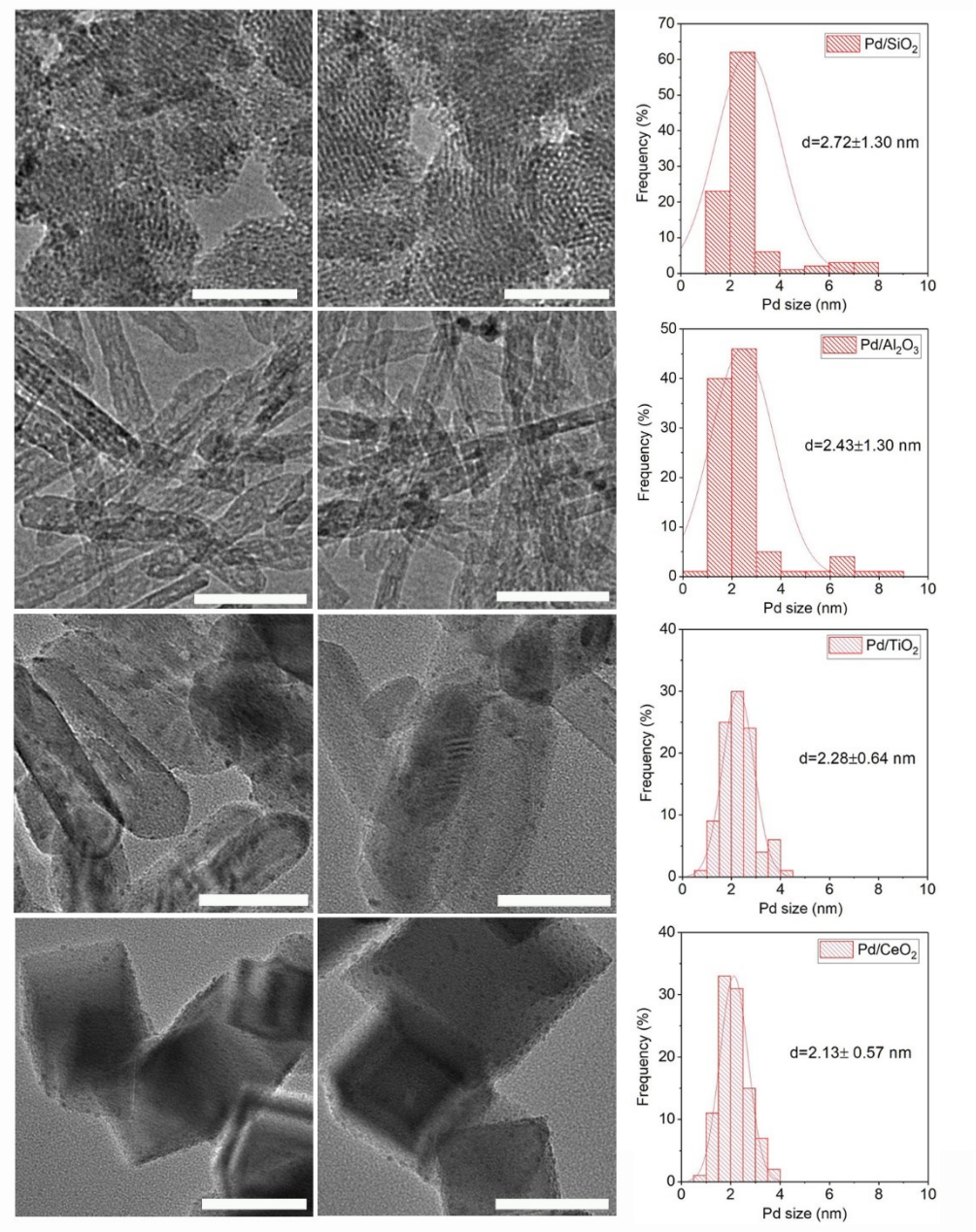

Figure S3. The TEM images of Pd/MO_x catalysts and the corresponding histogram of the particle size distribution. Scale bar is 20 nm.

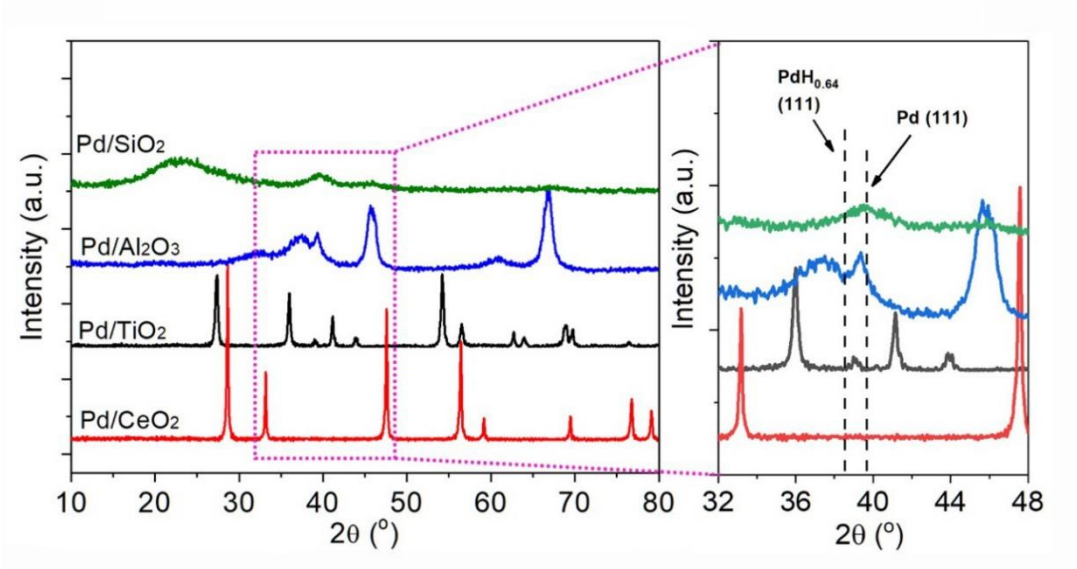

Figure S4. XRD patterns of Pd/SiO_2, Pd/Al_2O_3, Pd/TiO_2 and Pd/CeO_2, as well as enlarged patterns to analyze Pd crystal and $PdH_{0.64}$ crystal phases.

Note: According to XRD patterns of Pd/MO_x, peaks of silica, alumina, rutile TiO_2 and ceria were observed. The enlarged patterns do not show Bragg reflections of Pd (JCPDS 87-0641) resulting from the small size of the Pd species except for Pd/SiO_2, due to the much weak diffraction peaks of SiO_2 nanocrystals. The peaks of Pd (111) and PdH_x (111) are located at 39.6° and 38.7°, respectively, indicating with dot lines.

Table S1. The Pd loading of various Pd/MO_x catalysts.

samples	**Pd/SiO_2**	**Pd/Al_2O_3**	**Pd/TiO_2**	**Pd/CeO_2**
Pd loading (wt.%)	1.71	1.70	1.75	1.73

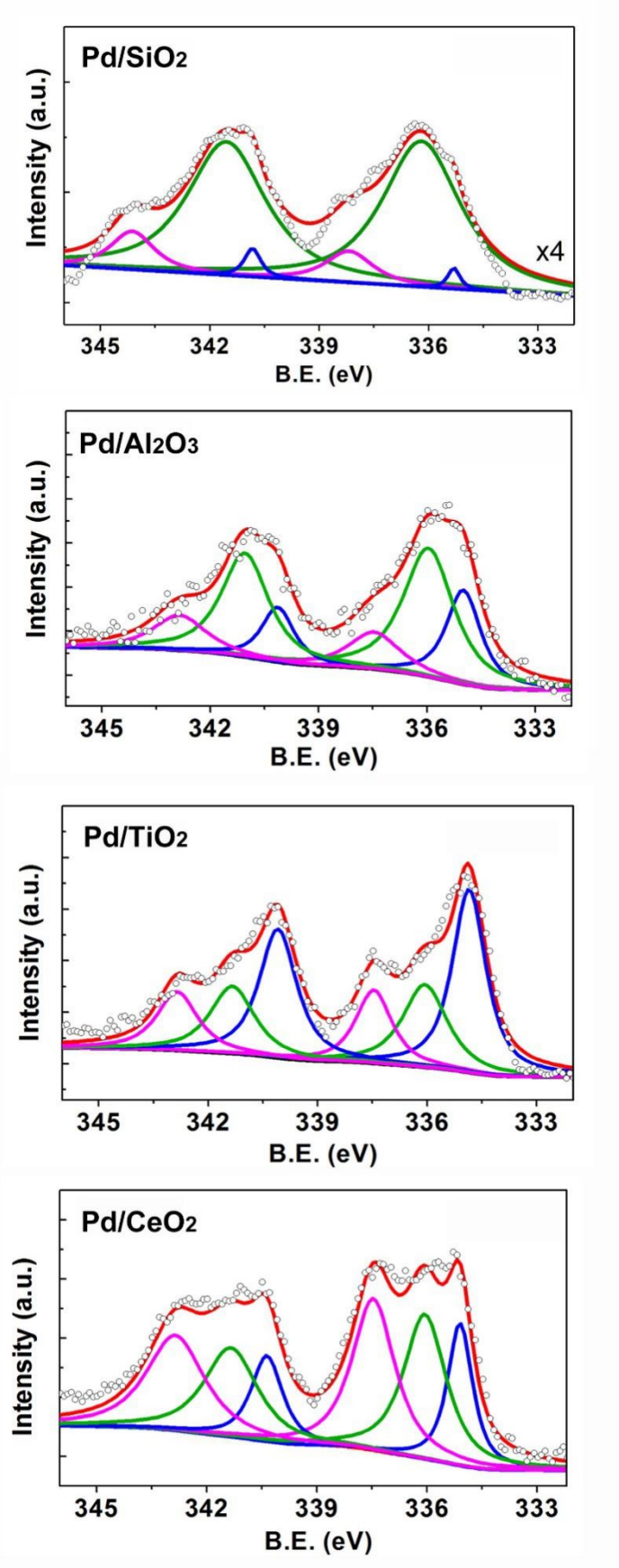

Figure S5. Pd 3d XPS profiles of Pd/MO_x catalysts.

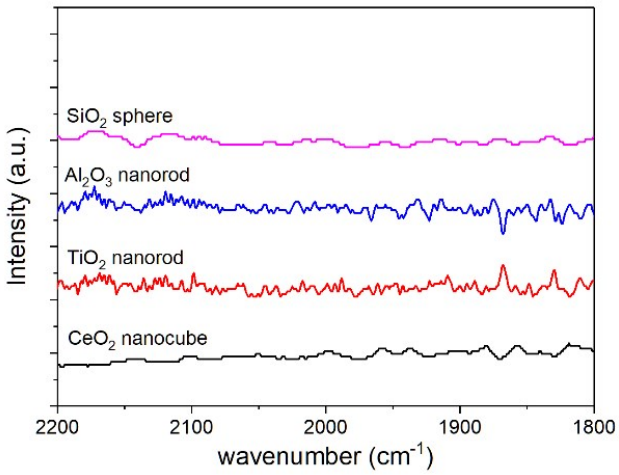

Figure S6. In situ DRIFTS spectra of CO chemisorption over MO_x at 25 °C. And no CO adsorption bands were observed on pure oxides.

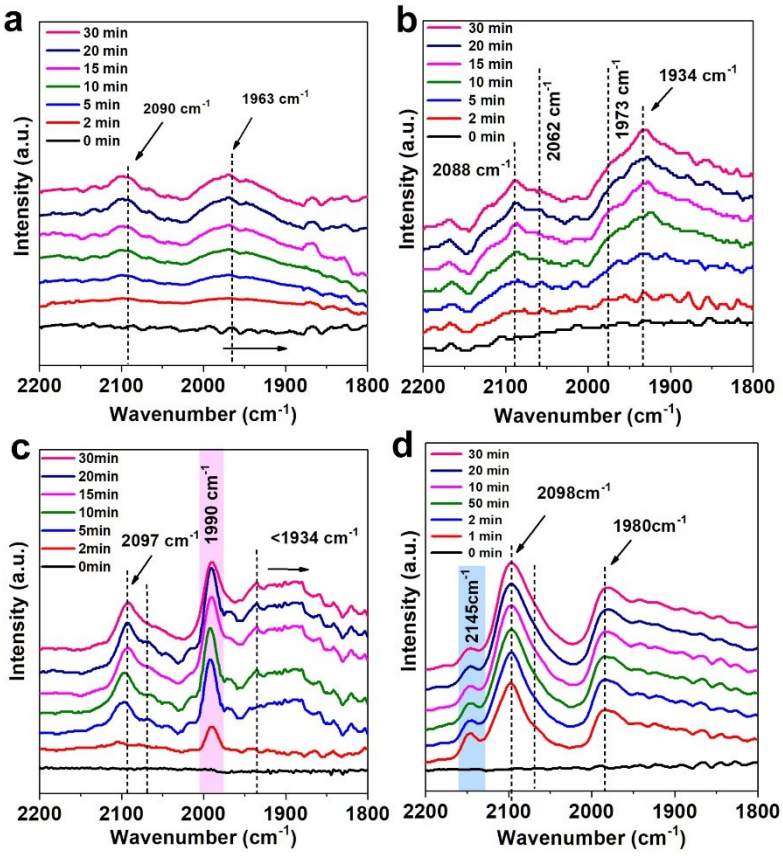

Figure S7. In situ DRIFTS spectra of CO chemisorption over Pd/MO_x at 25 °C: (a) Pd/SiO_2; (b) Pd/Al_2O_3; (c) Pd/TiO_2; (d) Pd/CeO_2. The Pd/MO_x catalysts were pretreated under Ar at 25 °C for 60 min and then collect spectra once exposed to CO/Ar atmosphere. The decreasing of saturated

adsorption time suggests that the CO adsorption strength increase from Pd/SiO_2 (~20min), Pd/Al_2O_3 (~15min) and Pd/TiO_2 (5min) to Pd/CeO_2(<2min).

More details of the CO adsorption structure and additional explanations:

Both linear and multi-coordinated CO_Pd^0 bands (CO adsorption on Pd^0 species) present in Pd/SiO_2 and Pd/Al_2O_3 clearly, because of a large amount of Pd^0 species exposing to surface (86.6% and 63.1%, respectively). As the surface Pd^0 species decreases, the peak intensity declines obviously in Pd/TiO_2. Even for Pd/CeO_2, there is not multi-coordinated CO_Pd^0, due to the dominant Pd^{2+} and $Pd^{\delta-}$ species on the surface.

For the CO_$Pd^{\delta-}$ bands (CO adsorption on $Pd^{\delta-}$ species), both linear and multi-coordinated CO_$Pd^{\delta-}$ present in Pd/Al_2O_3, Pd/TiO_2 and Pd/CeO_2, as the $Pd^{\delta-}$ species were primarily located on superficial, which is beneficial to the formation of multiple CO adsorption structures. It is generally accepted that the red-shift of the stretching wavenumber of adsorbed CO is indicative of an increasing electron donation from metals into the π* C=O orbital in the case of CO adsorption on electron-rich metal sites[1,2]. By analogy, the peak at 2066 cm^{-1} for Pd/TiO_2 also could be considered as a relative red-shifted peak from 2097 cm^{-1}. Furthermore, the red shift of 31 cm^{-1} (from 2097 cm^{-1} to 2066 cm^{-1}) is much larger than that of Ag@Pd NPs (11 cm^{-1})[2], poly(allylamine)-stabilized Pd (~20 cm^{-1})[1], and pyridinic-N-tuned Pd (<15 cm^{-1})[3], demonstrating that TiO_2 as a support promoted superficial Pd atoms to gather more electrons.

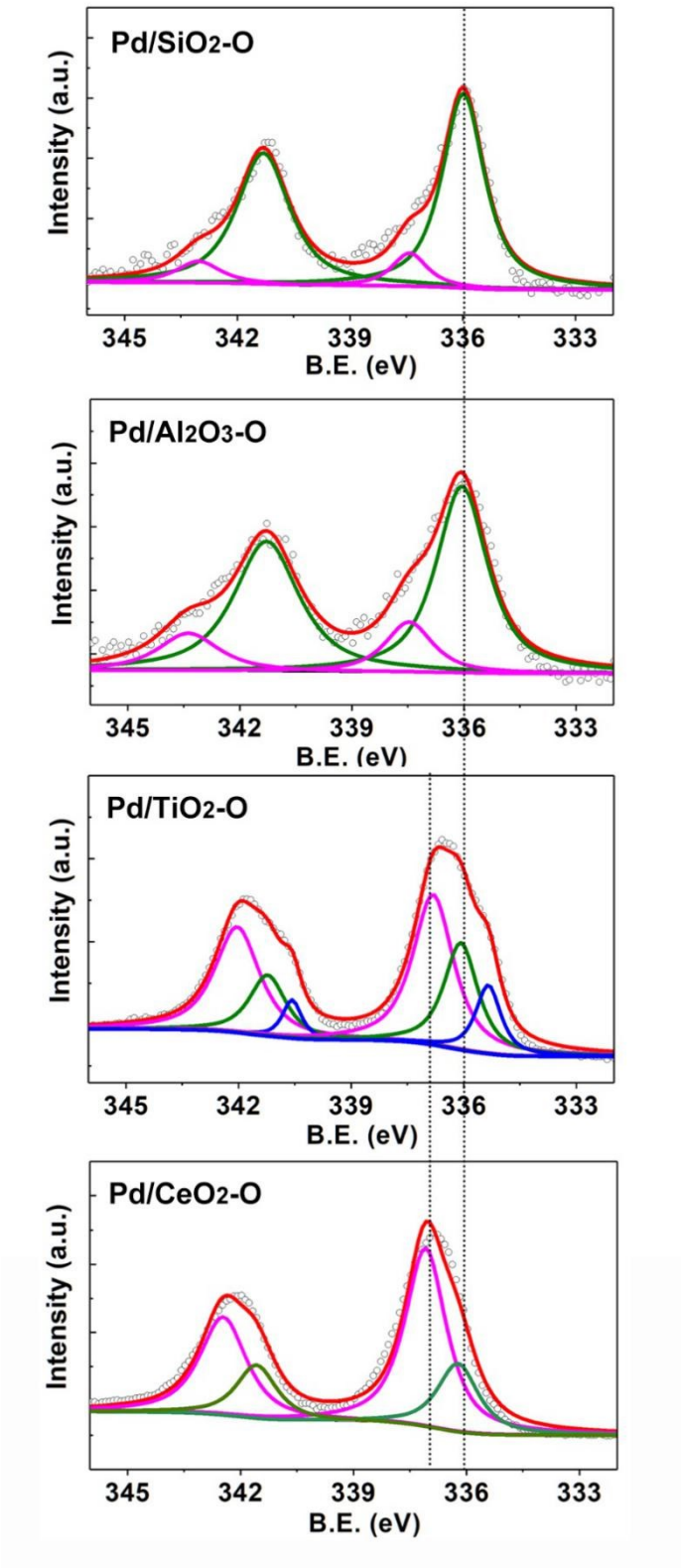

Figure S8. Pd 3d XPS profiles of Pd/MO_x after reoxidation treatment at 300°C under O_2/N_2 and followed by 5% H_2/Ar flushing for 30 min at 25 °C (denoted as Pd/MO_x-O).

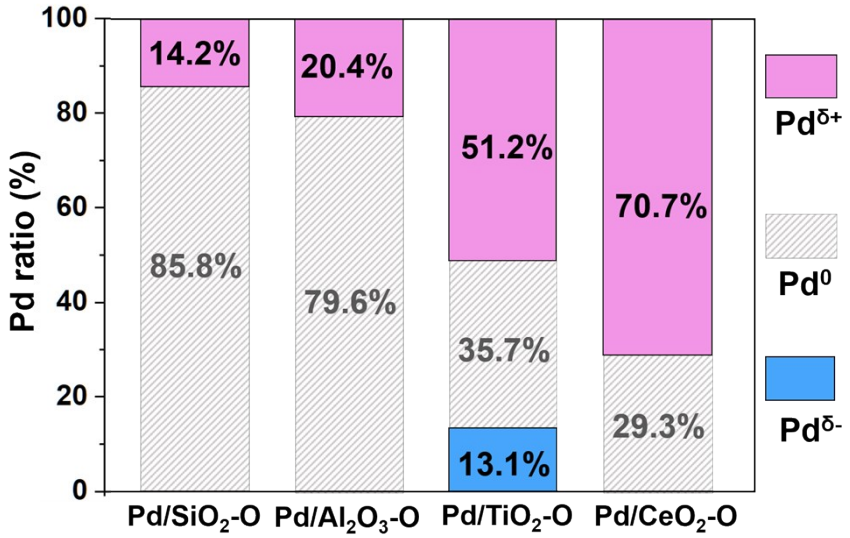

Figure S9. The relative proportions of $Pd^{\delta+}$, Pd^{0} and $Pd^{\delta-}$ species in Pd/MO_x-O.

Note: The Pd/MO_x samples were re-oxidized at 300 °C under O_2/N_2 and followed by 5% H_2/Ar flushing for 30 min at 25 °C (denotated as Pd/MO_x-O). As shown in Figure S8 and S9, metallic Pd is the dominant species for Pd/SiO_2-O and Pd/Al_2O_3-O (almost 85.8% and 79.6%, respectively). In the case of Pd/TiO_2-O, the multi-peak fitting for the asymmetric peak suggests that Pd^0, $Pd^{\delta-}$ and $Pd^{\delta+}$ species coexisted in the sample. Furthermore, the Pd^{2+} species in Pd/MO_x transform into $Pd^{\delta+}$ species in Pd/MO_x-O indicating that electrons partly transfer from the supports back to metals under oxidative conditions, and thus the *p*EMSI is weakened. Due to the strong interaction between Pd NPs and CeO_2, $Pd^{\delta+}$ species is dominant in Pd/CeO_2-O. However, in Pd/SiO_2-O and Pd/Al_2O_3-O, the absence of Pd^{-} species suggests that the *p*EMSI effect almost disappeared, due to the weak interaction between Pd NPs and SiO_2 or Al_2O_3.

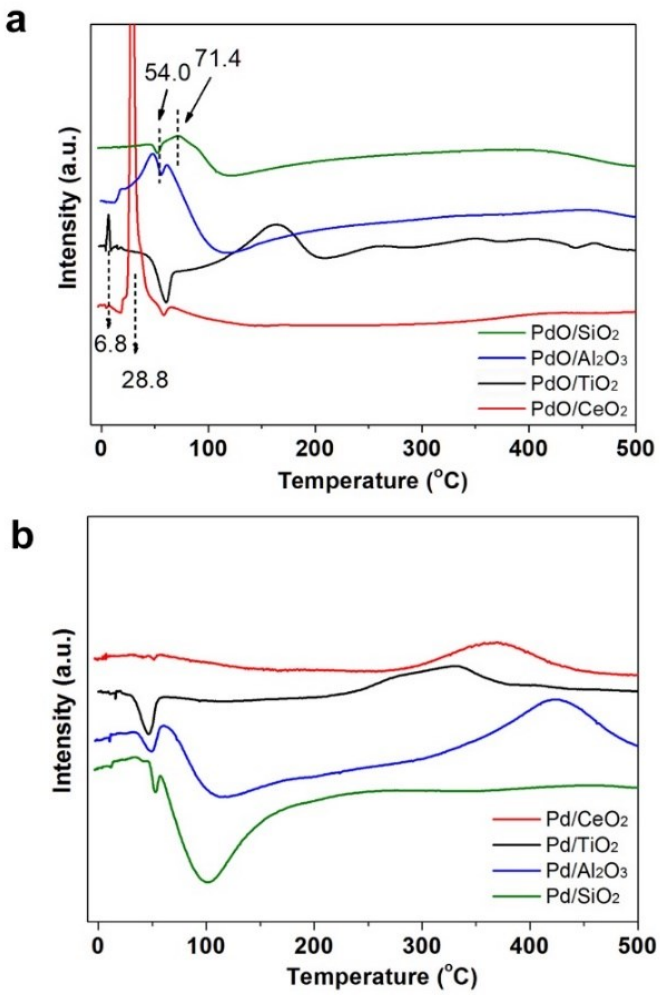

Figure S10. H_2-TPR profiles of (a) PdO/MO_x and (b) Pd/MO_x. Obviously, the PdO peaks appeared for PdO/MO_x, but those peaks were not detected in the Pd/MO_x catalysts.

Note: The PdO/MO_x samples were prepared by oxidation of the fresh Pd/MO_x samples under 20% O_2/N_2 atmosphere at 300 °C for 1 hour and cooling down to room temperature under the same atmosphere. H_2-TPR profiles were colected from ~0 to 500 °C. It is generally accepted that Pd species are relatively easy to be oxidized in air, so the origin of Pd^{2+} species were considered carefully. In comparison with PdO/MO_x (Figure S10a), the Pd/MO_x samples (Figure S10b) do not contain PdO species, and thus, all Pd^{2+} species in Pd/MO_x are derived from the charge transfer from Pd atoms to oxide supports.

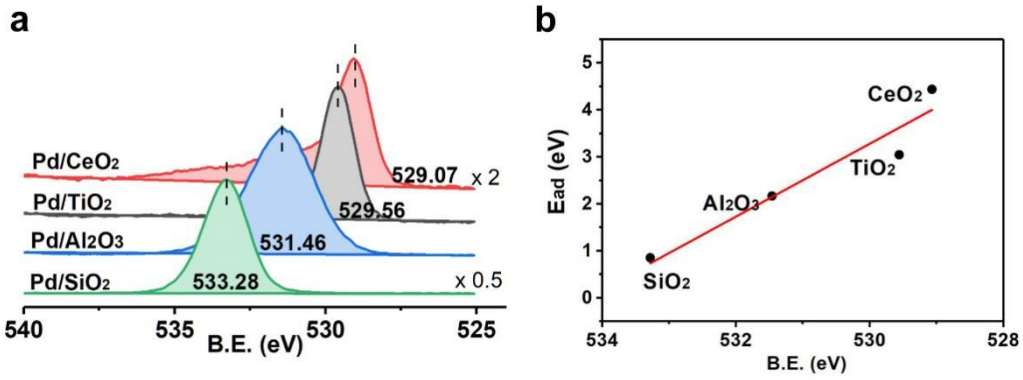

Figure S11. (a) O 1s XPS profiles of Pd/MO_x catalysts. (b) The correlation between adsorption energy (E_{ad}) and binding energy of O_{1s} (B.E.).

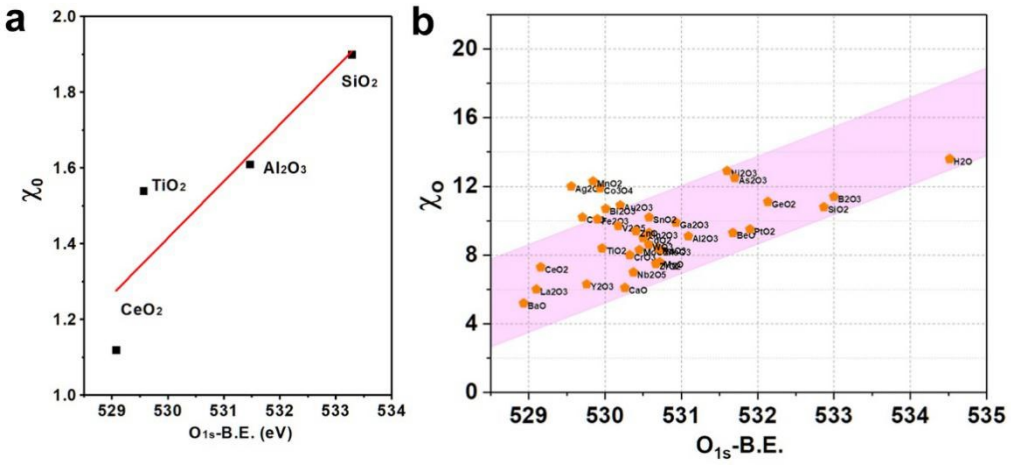

Figure S12. The correlation between binding energy of O_{1s} (BE) and the electronegativity of the central metal ion (χ_0) according to the table of the electronegativity of atoms coined by Roald Hoffmann[4,5] (a) experimental oxides, the BE of O_{1s} obtained from O 1s XPS profiles of Pd/MO_x catalysts. (b) reference oxides, all data of O_{1s} BE were compiled from the NIST X-ray Photoelectron Spectroscopy Database[5] by taking the mean value of O_{1s} BE as the input values.

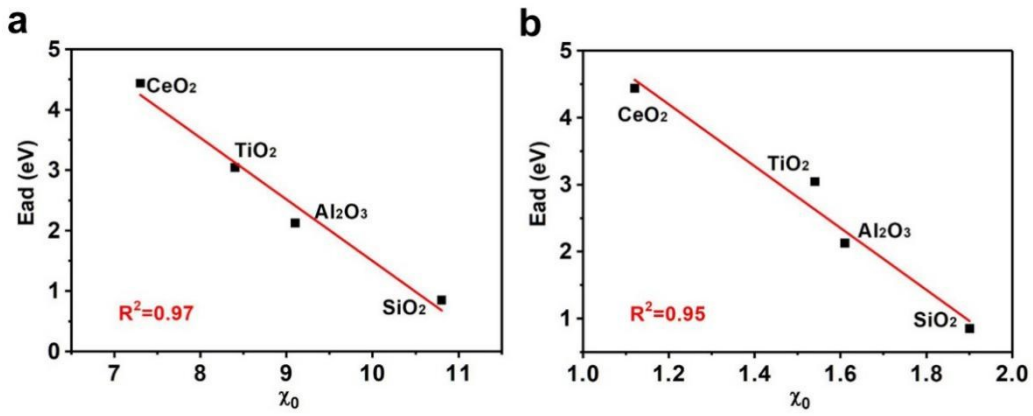

Figure S13. (a) The correlations between adsorption energy (E_{ad}) and the electronegativity of the central metal ion (χ_0) according to the table of the electronegativity of atoms coined by Roald Hoffmann; (b) The correlation between adsorption energy (E_{ad}) and the electronegativity of the central metal ion in Pauling scale ($\chi_{0\text{-}p}$).

Note: The electronegativity of the central metal ion (χ_0) was introduced as a key factor, and the calculated E_{ad} was adopted as the descriptor of EMSI based on DFT calculations to better quantitatively describe and understand how to improve the electronic interaction. Surprisingly, the strong correlations among adsorption energy (E_{ad}), binding energy of O_{1s} and the electronegativity of the central metal ion (χ_0) were revealed (Figure S10, S11 and S12)[4].

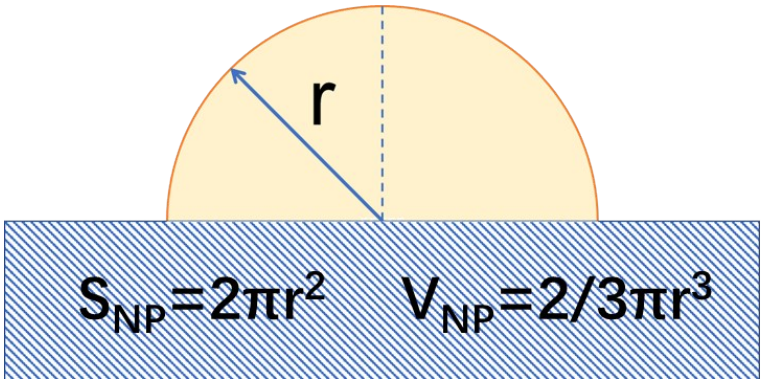

Figure S14. The model of supported Pd nanoparticle, the surface area and volume of nanoparticle in order to calculate metal dispersions for Pd/MO_x.

Note: The number of surface Pd atoms were calculated by calculated metal dispersion (D). The calculated dispersion can be expressed as $D=(S_{NP}*N_s)/ (V_{NP}*N_v)^6$, where S_{NP} and V_{NP} represent the surface area and volume of supported Pd nanoparticles, respectively (Figure S14); N_s (15.25 atoms/nm^2) and N_v (67.92 atoms/nm^3) represent the number of atoms per unit volume and per unit area based on the bulk Pd crystalline structure, respectively. The radii of supported Pd NPs were derived from the histograms of the particle size distributions (Figure S3).

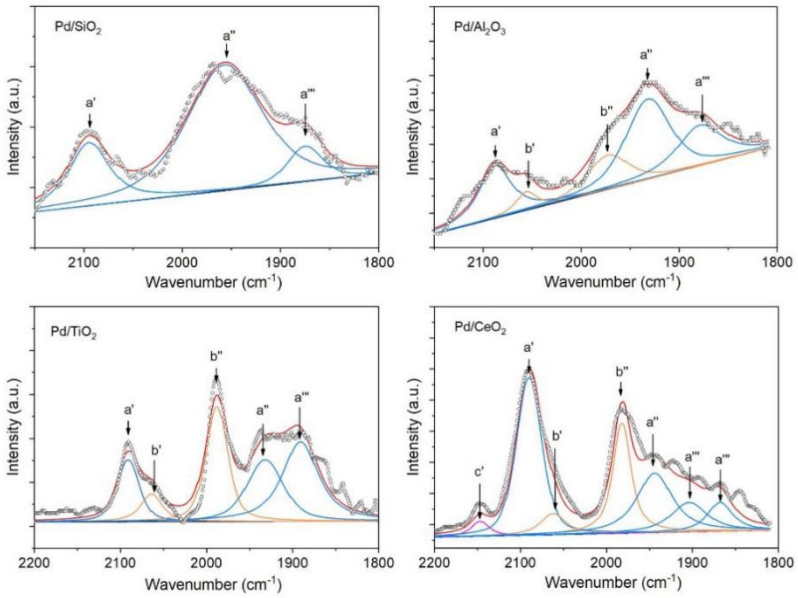

Figure S15. DRIFTS spectra of CO adsorption on Pd/MO_x catalysts at RT and corresponding peak-fitting results in order to calculate the number of surface $Pd^{\delta-}$ atoms for Pd/MO_x. The solid lines and scatter data represent the fitted curves and original data, respectively. a', a'' and a''' are the adsorption peaks of linear CO, bridge CO and three-fold CO on Pd^0 atoms, respectively. b' and b'' are the adsorption peaks of linear CO, bridge CO on $Pd^{\delta-}$ atoms, respectively. c' is the adsorption peak of linear CO on Pd^{2+} atoms.

Note: Based on the detailed assignment of the C-O stretching vibration characteristic peaks of absorbed CO (Figure 4), the deconvolution of the DRIFT spectra was performed for a quantitative analysis. The surface concentration (C) of the adsorbate is proportional to a simple function of R ($C \propto R$, R= $I_{cat+ads}/I_{cat}$), where the intensity $I_{cat+ads}$ and I_{cat} are measured over the catalyst in the presence of the adsorbate and free of adsorbates[7].Here, we applied the peak area (A) as the intensity. As the baseline data, the I_{cat} for all peaks are constant in this system, i.e., R=constant* $I_{cat+ads}$. So, the surface concentration then is proportional to $I_{cat+ads}$($C \propto I_{cat+ads}$). Considering the adsorption structures, a'' and b'' are bridge CO on surface Pd atoms, which results in two surface Pd atoms occupied by a single CO molecule. Similarly a''' means that a single CO molecule occupies three Pd atoms. The areas of a'', b'' and a''' peaks should be multiplied by a coefficient of 2, 2 and 3, respectively, to measure the number of surface Pd atoms.

So, the ratio of surface $Pd^{\delta-}$ atoms (at%$Pd^{\delta-}$) can be expressed as:

$$at\%Pd^{\delta-}=(A_{b'}+A_{b''}*2)/(A_{a'}+A_{b'}+A_{c'}+A_{a''}*2+A_{b''}*2+A_{a'''}*3+A_{b'''}*3)$$

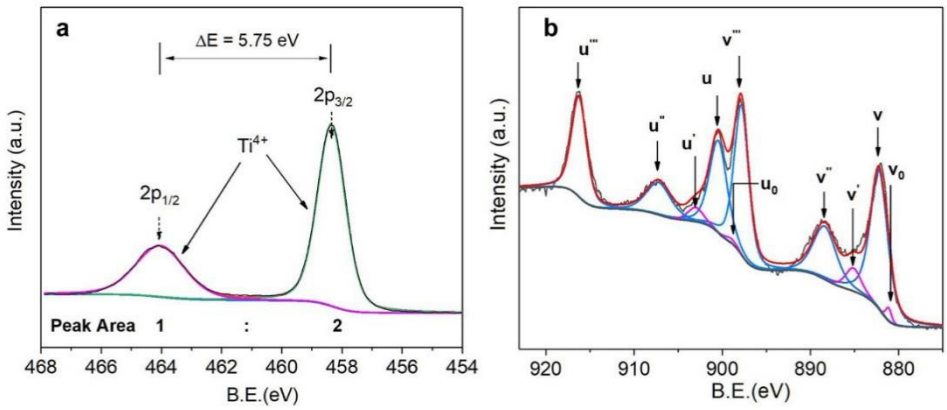

Figure S16. XPS spectra and corresponding peak fitting of (a) Ti2p in Pd/TiO_2 and (b) Ce3d in Pd/CeO_2.

Table S2. Intensities (calculated peak areas), inter-component intensity ratios for peaks relevant to Ce^{3+} and Ce^{4+} species derived from the curve-fitting of the XPS Ce3d spectrum (Figure 5.) $I_{tot}Ce^{3+}$ and $I_{tot}Ce^{4+}$ represent the total intensities of Ce^{3+} and Ce^{4+} related peaks, respectively. Relative errors are reported, which referred to the theoretical intensity ratio of 1.5 in Ref.[8,9].

Intensity， $I_{tot}Ce^{3+}$ = 2.53*10^4			
I_v^o	I_v'	I_u^o	I_u'
0.28*10^4	1.27*10^4	0.19*10^4	0.78*10^4
Inter-component ratio			
I_v^o/I_u^o	I_v'/I_u'		$\sum I_v^i/I_u^i$
1.49(0.67%)	1.63(8.67%)		1.60(6.67%)

1.50	1.50			1.50	
Intensity， $I_{tot}Ce^{4+}$ = 34.6*10^4					
I_v	I_v''	I_v'''	I_u	I_u''	I_u'''
8.87*10^4	4.32*10^4	7.66*10^4	5.70*10^4	2.81*10^4	5.28*10^4
Inter-component ratio					
I_v/I_u	I_v''/I_u''	I_v'''/I_u'''		$\sum I_v^i/I_u^i$	
1.55(3.33%)	1.54(2.67%)	1.45(3.33%)		1.51(0.67%)	
1.50	1.50	1.50		1.50	

Note: Quantitative analysis of XPS spectra (Ti2p and Ce3d) was performed applying peak fitting (Figure S16 and Table S2). The formation of any surface oxygen defects triggers the reduction of Ti^{4+} to Ti^{3+} and Ce^{4+} to Ce^{3+}. And the relative concentration of Ti^{3+} and Ce^{3+} can be calculated by the area of XPS deconvolution peaks. For Pd/TiO_2, the peak area ratio (1:2) and doublet separation energy for Ti2p XPS peaks (5.75 eV) were determined to agree well with the theoretical values, 1:2 and 5.76 eV, respectively (Figure S16a)[10], indicating that the only Ti^{4+} existed in the Pd/TiO_2 catalysts. Because of the spectral complexity of Ce3d XPS spectra for cerium oxides, inter-component peak intensity ratios are concerned in the peak fitting to evaluate the accurate Ce^{3+} percentage (Figure S16b). Theory suggests that each of the two spin-orbit split components of the Ce3d subshell contains 10 electrons, which distributed into n_{j+} (6-fold degenerate electrons) and n_{j-} (4-fold degenerate electrons) resulting in their intensity ratio of 6/4 (= 1.5) [8]. That is, each of the XPS $Ce3d_{5/2}$ peaks is 1.5 times as intense as the corresponding $Ce3d_{3/2}$ peak, and similarly the ratio of the summation of the intensities of $Ce3d_{5/2}$ peaks to $Ce3d_{3/2}$ peaks is 1.5. As shown in Table S2, the inter-component peak intensity ratios were calculated, and the relative errors are also shown in parenthesis, all of which are within 10%.

Therefore, the at%[Ce3+] percentage is:

$$\text{at\%}[Ce^{3+}] = \frac{I_{tot}Ce^{3+}}{I_{tot}Ce^{3+} + I_{tot}Ce^{4+}} \times 100 = \frac{2.53}{2.53 + 36.4} \times 100 = 6.5$$

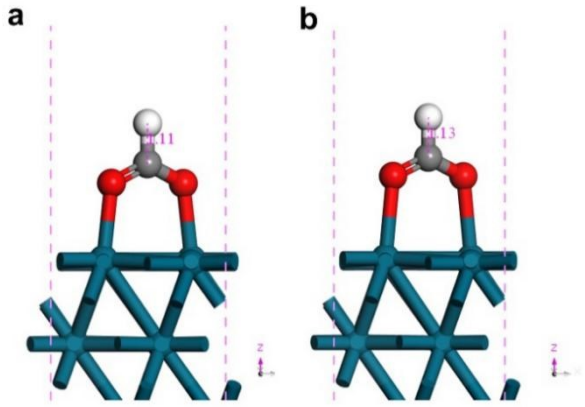

Figure S17. The interactions of bridging formate on the surface of Pd(111): (a) neutral HCOO*-Pd(111), (b) electron-riched HCOO*-Pd(111) with extra 2*e*.

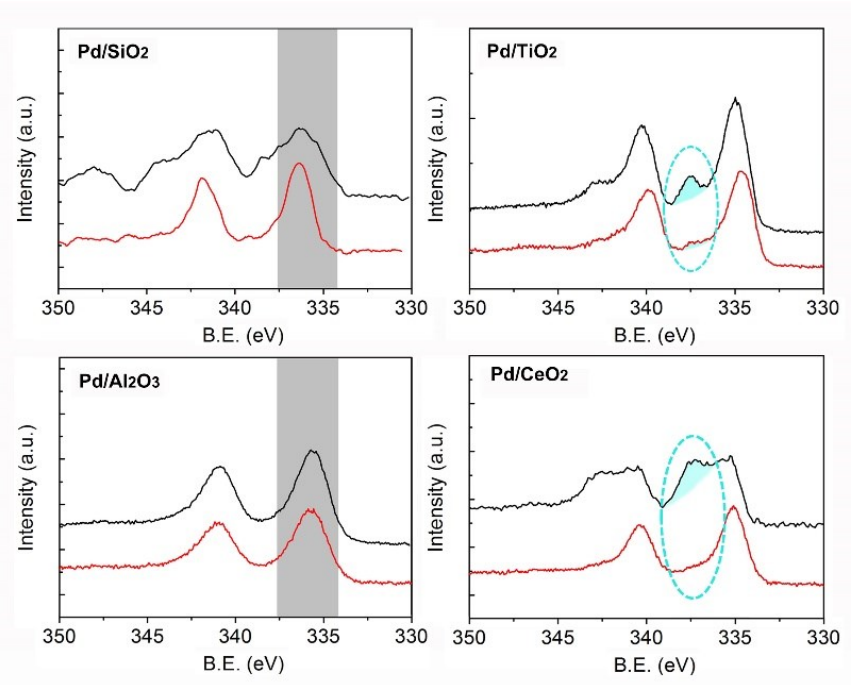

Figure S18. Pd 3d XPS profiles for Pd/MO_x catalysts before (black line) and after (red line) usage.

2. References

1 Jones, S.; Qu, J.; Tedsree, K.; Gong, X. Q.; Tsang, S. C. *Angew. Chem. Int. Ed.* **2012,** *51* (45), 11275.

2 Tedsree, K.; Li, T.; Bagot, P. A. J.; Jones, S.; Marquis, E. A.; Chan, C. A.; GeorgeD.W.Smith; Yu, K. M. K.; Tsang, S. C. E. *Nat. Nanotechnol.* **2011,** *6*, 302.

3 Bi, Q. Y.; Lin, J. D.; Liu, Y. M.; He, H. Y.; Huang, F. Q.; Cao, Y. *Angew. Chem. Int. Ed.* **2016,** *55* (39), 11849.

4 Rahm, M.; Zeng, T.; Hoffmann, R. *J. Am. Chem. Soc.* **2019,** *141*, 342.

5 In *Version 4.1*, DOI:http://dx.doi.org/10.18434/T4T88K.

6 Anderson, J. R. *Structure of metallic catalysts / J. R. Anderson*; Academic Press: London ; New York, 1975.

7 Sirita, J.; Phanichphant, S.; Meunier, F. C. *Anal. Chem.* **2007,** *79* (10), 3912.

8 Paparazzo, E. *Applied Catalysis B: Environmental* **2011,** *105* (1-2), 248.

9 Anandan, C.; Bera, P. *Appl. Surf. Sci.* **2013,** *283*, 297.

10 Georgiadou, I.; Spanos, N.; Papadopoulou, C.; Matralis, H.; Kordulis, C.; Lycourghiotis, A. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **1995,** *98* (1), 155.

3. Appendix

Calculated Cartesian coordinates of all calculated structures:

SiO2_001_Pd4

1.0

10.0439996719	0.0000000000	0.0000000000
5.0219998360	8.6983588715	0.0000000000
-0.0000048647	-0.0000028086	36.5330009460

O	Si	Pd
80	40	4

Cartesian

4.156377792	2.100079536	0.487277150
2.853750706	3.254629612	6.305084229
3.173595905	3.130198956	11.596085548
4.981562138	3.356087208	2.671220064
4.835788727	3.683049440	8.046174049
4.809085369	3.288883209	13.787700653
0.944426656	0.545769453	4.309542656
1.126583934	0.784191012	9.965509415
2.716127872	1.598966837	2.688061714
3.035526514	1.823627710	8.514527321
2.676753998	1.776708245	13.807428360
5.961479664	4.444069386	4.871346951
6.156001091	4.229358673	10.252511978
2.211834431	0.339801341	0.379870117
4.873197079	1.511896014	6.571227074
4.794054985	1.168493032	12.249404907
3.976356983	2.218010664	16.092933655

1.998869419	0.444337010	15.986767769
6.490591526	3.048199415	15.835155487
6.672274113	2.928676367	0.630924940
9.178377151	2.100079536	0.487277150
7.875750542	3.254629612	6.305084229
8.191794395	3.130973339	11.587208748
10.003561974	3.356087208	2.671220064
9.857788086	3.683049440	8.046174049
9.830181122	3.301269531	13.774330139
5.966426373	0.545769453	4.309542656
6.149693489	0.771447957	9.973107338
7.738128185	1.598966837	2.688061714
8.057526588	1.823627710	8.514527321
7.681553364	1.795157433	13.795409203
10.983479500	4.444069386	4.871346951
11.180829048	4.230132580	10.252621651
7.233834267	0.339801341	0.379870117
9.895196915	1.511896014	6.571227074
9.814406395	1.173259735	12.248639107
9.006065369	2.189819336	16.049642563
6.999731541	0.455253482	15.980703354
11.523961067	3.042510509	15.833804131
11.694273949	2.928676367	0.630924940
6.667377472	6.449258804	0.487277150
5.364750385	7.603808880	6.305084229
5.684440136	7.482083321	11.586988449
7.492561817	7.705266953	2.671220064
7.346788406	8.032228470	8.046174049

7.312913895	7.640741825	13.785471916
3.455426693	4.894948959	4.309542656
3.638658285	5.131612778	9.972413063
5.227128029	5.948146343	2.688061714
5.546526909	6.172807217	8.514527321
5.170342445	6.144841194	13.793948174
3.450479746	0.094890021	4.871346951
8.667367935	8.578372002	10.253535271
4.722834587	4.688980579	0.379870117
7.384197235	5.861075401	6.571227074
7.302488804	5.522030354	12.248456001
6.442756653	6.590405464	16.074264526
4.475559235	4.797012806	15.956007957
8.981840134	7.376980782	15.847249031
9.183273315	7.277855396	0.630924940
11.689377785	6.449258804	0.487277150
10.386750221	7.603808880	6.305084229
10.686843872	7.467435837	11.601821899
12.514561653	7.705266953	2.671220064
12.368788719	8.032228470	8.046174049
12.316945076	7.638827801	13.792633057
8.477425575	4.894948959	4.309542656
8.658905983	5.129986763	9.964741707
10.249128342	5.948146343	2.688061714
10.568526268	6.172807217	8.514527321
10.192870140	6.122791290	13.824087143
8.472478867	0.094890021	4.871346951
13.690688133	8.581286430	10.253023148

9.744833946	4.688980579	0.379870117
12.406196594	5.861075401	6.571227074
12.314533234	5.515715122	12.255067825
11.487481117	6.582411766	16.107437134
9.557938576	4.770161152	15.996230125
14.002001762	7.403110504	15.836398125
14.205273628	7.277855396	0.630924940
2.674952745	1.748691797	1.049994946
3.895885706	2.559456587	7.349452972
3.861328602	2.352983236	12.840728760
5.138826847	3.259196758	1.040679097
4.926992416	0.263559848	5.522803307
5.056805611	0.154821232	11.011740685
4.949224472	3.339672565	15.426607132
2.406993866	0.313488573	3.652678967
2.529806137	0.448217005	9.210737228
2.525983334	1.870824337	15.438261986
7.696952820	1.748691797	1.049994946
8.917885780	2.559456587	7.349452972
8.876910210	2.358324051	12.835175514
10.160825729	3.259196758	1.040679097
9.948991776	0.263559848	5.522803307
10.080779076	0.165233165	11.005273819
9.989403725	3.311924934	15.409619331
7.428993702	0.313488573	3.652678967
7.551805973	0.448217005	9.210737228
7.536664009	1.874982119	15.426973343
5.185953140	6.097871304	1.049994946

6.406886101	6.908636093	7.349452972
6.366055489	6.707355499	12.834372520
7.649827003	7.608376026	1.040679097
7.437992573	4.612739086	5.522803307
7.568357944	4.512577057	11.004798889
7.458827972	7.690661430	15.419118881
4.917994022	4.662667751	3.652678967
5.040805817	4.797396660	9.210737228
4.987747669	6.228371620	15.417949677
10.207952499	6.097871304	1.049994946
11.428885460	6.908636093	7.349452972
11.373637199	6.694020748	12.848730087
12.671826363	7.608376026	1.040679097
12.459992409	4.612739086	5.522803307
12.591406822	4.510254383	11.011667252
12.463893890	7.693966866	15.429968834
9.939992905	4.662667751	3.652678967
10.062806129	4.797396660	9.210737228
10.042330742	6.221691608	15.454445839
9.002478600	4.703731537	18.426149368
6.696613312	3.372317314	18.550107956
6.726112843	6.027577877	18.404924393
7.513707161	4.808059692	20.517080307

Al2O3_110_Pd4

1.0

8.4130001068	0.0000000000	0.0000000000
-0.0830810040	8.0675720611	0.0000000000

-0.0000083582 -0.0000084447 31.3845996857

O Al Pd

54 36 4

Cartesian

3.586626768	7.386300564	3.084462643
3.475185156	7.316686630	8.594333649
7.764607906	5.055858135	1.363234043
7.858466625	5.042865276	7.026563168
3.634816647	6.819906712	31.046518326
3.509095430	6.979537487	5.639062405
3.609799862	6.915192604	11.127192497
7.847551346	5.230297565	4.375734806
7.739969730	5.141276360	10.135182381
7.791420937	0.997646034	4.283862591
7.814534187	0.918891370	9.714748383
3.707256317	3.454153299	31.380043030
3.643911123	3.221771717	5.814198017
3.675211668	3.180218220	11.615566254
7.826588631	1.263450623	1.678285122
7.779827118	1.263678312	7.152942657
3.569523096	2.988148928	2.545871735
3.651081562	2.987327576	8.448247910
5.184673309	0.989071906	4.284983158
5.133564949	0.914365470	9.714937210
0.795745194	3.459688187	31.368173599
0.833327234	3.218340635	5.813548088
0.859009624	3.193271637	11.635623932
5.133209705	1.249322653	1.679446340

5.150142193	1.257222652	7.151037216
0.992791414	2.983229160	2.514618874
0.852518022	2.985610485	8.452035904
0.817676127	7.383386612	3.089047909
0.904438376	7.311212540	8.598106384
5.164542198	5.049097061	1.354506016
5.019817352	5.038904667	7.021933556
0.870002568	6.810054779	31.035957336
0.920474291	6.976758003	5.644272327
0.785411656	6.893731117	11.136332512
5.003284454	5.221014500	4.367151260
5.080533028	5.140638351	10.147761345
6.417251587	7.201321602	2.986731052
6.403200626	7.104136467	8.556019783
6.445204735	7.382108212	0.063161507
6.416224003	7.264731407	5.644582748
6.402105331	7.448391438	11.192539215
2.273103237	1.209564328	4.184901237
2.261308908	1.084185481	9.899195671
2.279778957	1.026760340	1.215170860
2.261082172	0.979569912	7.164696217
2.258147240	5.143971443	1.436096549
2.228295088	5.235914230	7.052637577
2.222683907	5.145849705	4.394016743
2.216467381	5.024976730	9.997702599
6.465786457	2.743383408	0.164634198
6.450847626	3.024502039	5.761845112
6.474888802	2.805603027	11.386395454

6.469654560	3.118436098	2.831421137
6.449110985	3.081588984	8.448310852
0.755135894	5.255458832	0.351209372
0.741503894	5.061497688	5.692746162
0.734768033	4.954124451	11.196961403
4.972984314	7.064179897	4.276961327
5.022888660	6.993644714	9.951696396
5.085659027	3.198811769	1.342102766
4.998538971	3.207844496	7.145146370
0.797528028	1.136452198	2.954630852
0.810383499	1.141574502	8.497085571
7.842706203	3.205554008	1.344999552
7.907613754	3.214948654	7.163873672
3.760489702	1.144398689	2.973822594
3.716668129	1.146310925	8.500176430
3.757345676	5.257863045	0.350562841
3.708260298	5.070638180	5.705045700
3.685755730	4.916461468	11.244527817
7.854796410	7.071671963	4.290629387
7.779335022	7.005092621	9.954621315
6.479490757	0.963710845	0.412776530
6.478236198	1.127420545	5.713233471
6.470347881	1.160296082	10.993563652
6.485505581	1.180179238	3.001732826
6.466584206	1.047617078	8.416771889
6.461200714	6.267337322	1.385357022
6.435180664	6.089598179	7.071716309
2.247492313	7.603466988	0.264113963

2.201456070 7.117156506 7.123779774

2.207314491 7.121204376 4.245165825

2.195491314 7.181792736 10.009132385

2.246194601 2.768836260 0.762008667

2.241756678 2.144264698 5.745889187

2.273975611 2.375746012 11.102028847

2.275768995 4.177021503 2.956074476

2.250195265 4.086599350 8.436374664

6.433866501 4.158025265 4.309102058

6.411046505 3.955878735 10.088169098

3.465080976 6.445006847 13.261552811

2.217772722 5.780623913 15.410660744

1.840300083 4.239013672 13.386887550

0.856233895 6.662642956 13.380261421

TiO2_110_Pd4

1.0

8.8769998550 0.0000000000 0.0000000000

-0.0000034605 12.9937896729 0.0000000000

-0.0000077351 -0.0000077351 29.0448207855

O Ti Pd

72 36 4

Cartesian

0.000011795 -0.000007734 29.041769028

8.876978874 6.496884346 29.041770935

2.958992243 -0.000007734 29.041753769

2.958998442 6.496886253 29.041782379

5.917977810 -0.000007734 29.041769028

5.917997837	6.496884346	29.041769028
0.005273876	3.281103611	3.196702003
0.005771920	9.756334305	3.221056223
2.988711596	3.270154953	3.218035460
2.959222317	9.759776115	3.219990015
5.892809868	3.270953178	3.218322992
5.927707672	9.760282516	3.219740391
8.841572762	0.059989296	6.491363525
8.871250153	6.608335018	6.518944263
2.915585995	12.955182076	6.484014988
2.953367472	6.652069569	6.511393070
5.914141178	12.951030731	6.468560219
5.907949448	6.669470310	6.489243031
-0.000000684	-0.000000684	2.569206238
-0.000002414	6.496893406	2.569194317
2.958996058	-0.000000684	2.569182873
2.958998919	6.496894360	2.569206238
5.917990685	-0.000000684	2.569208860
5.917998791	6.496894360	2.569185734
0.007151583	3.221618891	5.759959698
0.009202179	9.755033493	5.855810642
2.918358326	3.256949186	5.818537235
2.970867395	9.752405167	5.845304966
5.977407455	3.253937006	5.818212032
5.924060822	9.747634888	5.845793247
0.054008797	0.032410596	9.070581436
0.048728794	6.527718544	9.095097542
3.039794922	0.121275119	9.068589211

2.988826752	6.386767387	9.087148666
5.932924271	0.112951294	9.052605629
5.944863796	6.383657932	9.062378883
1.479498863	4.456752300	1.050080657
1.479498148	10.953649521	1.050077796
4.438499928	4.456756115	1.050080657
4.438505650	10.953674316	1.050127029
7.397498131	4.456749439	1.050071955
7.397496700	10.953687668	1.050179362
1.481321096	1.313689113	4.499327660
1.477838755	7.844652176	4.508900642
4.438537598	1.311802506	4.553513527
4.436897755	7.846281528	4.491291046
7.393132687	1.314663768	4.491679668
7.401738644	7.844736576	4.504354954
1.430698276	4.534568310	7.861828804
1.509473681	10.998265266	8.026260376
4.462301731	4.561931610	7.607636929
4.465259075	10.978797913	8.026571274
7.493919849	4.530585766	7.867994785
7.414839745	10.995962143	8.022087097
1.479498506	2.040136576	1.050074816
1.479499459	8.537034988	1.050077796
4.438501835	2.040138960	1.050074816
4.438497066	8.537038803	1.050074816
7.397498608	2.040098667	1.050176501
7.397496700	8.537038803	1.050068974
1.480198026	5.220508575	4.553951740

1.471672654	11.671679497	4.530718803
4.440903664	5.222813129	4.579154491
4.437708855	11.671064377	4.514177799
7.400137424	5.221979141	4.553255081
7.405288696	11.670433998	4.527117252
1.511591434	2.092144728	8.008754730
1.508498788	8.583774567	8.074910164
4.460468292	2.040304899	7.756601810
4.458480358	8.565526009	8.080768585
7.421572208	2.090573788	8.016591072
7.418392181	8.579376221	8.079536438
-0.000001229	3.248436451	1.366698265
-0.000002959	9.745351791	1.366695404
2.958998442	3.248441696	1.366695404
2.958999395	9.745344162	1.366695404
5.918002129	3.248434067	1.366695404
5.918002129	9.745353699	1.366698265
0.015036535	12.960426331	4.510135174
0.007154610	6.460458755	4.483770847
2.978718996	12.970965385	4.504064560
2.960331917	6.471531868	4.481348515
5.928092957	12.963075638	4.488107681
5.929165840	6.464658737	4.464970589
0.025692483	3.228867769	7.581778526
0.020959258	9.811133385	7.708048344
2.974247217	3.393791199	7.930763721
2.976663589	9.789230347	7.695776939
5.949520588	3.377269745	7.924521923

5.945818901	9.770830154	7.697246552
1.479500055	-0.000000291	1.092294455
1.479494691	6.496891499	1.092276931
4.438509941	-0.000000291	1.092294455
4.438498497	6.496891499	1.092279911
7.397504330	-0.000000291	1.092271090
7.397509098	6.496894360	1.092303038
1.539546728	3.193821669	4.508502483
1.488355756	9.720085144	4.532830715
4.448624134	3.213570833	4.714166164
4.448429585	9.713326454	4.523495674
7.357898712	3.188255072	4.503500938
7.409200191	9.715070724	4.534050465
1.608223557	0.075383946	7.969324112
1.553978801	6.563497543	7.933455944
4.563691139	0.012053546	7.858645439
4.546891212	6.576210976	7.790886879
7.520062447	0.068807788	7.959501266
7.547746181	6.549422741	7.938919544
5.754799843	4.650426388	10.313879967
4.462348461	2.290805101	9.895799637
3.193104267	4.656729698	10.330072403
4.481328011	3.309069157	12.209053993

CeO2_100_Pd4

1.0

11.6406602859	0.0000000000	0.0000000000
-0.0000062002	11.6406602859	0.0000000000

-0.0000150368 -0.0000150368 28.2311897278

O Pd Ce

54 4 27

Cartesian

11.640538216	0.000934399	2.834597826
0.000335165	3.883974791	2.834857702
0.000505381	7.761735916	2.835230112
3.879990101	0.000582851	2.835746765
3.880111456	3.879341841	2.835187912
3.880350351	7.762204647	2.834075451
7.761276245	0.001398863	2.832048416
7.760268688	3.881731749	2.832471848
7.759448528	7.761775494	2.832017422
0.055436693	0.103070334	7.926372051
0.061633270	3.990561724	7.929443836
0.068911277	7.869951248	7.934516907
3.915889263	11.374185562	8.026640892
4.172091484	3.973444462	8.056794167
3.687893629	7.743387222	8.033198357
7.759673595	11.612403870	7.949361324
7.514908791	3.741704464	8.002122879
8.083173752	7.815333843	7.978286743
1.918997288	1.942014098	5.596918106
1.920999765	5.833542824	5.614638805
1.912726998	9.695086479	5.591486454
5.853621006	1.925180554	5.557594776
5.844498158	5.834518433	5.578113079
5.852842808	9.688963890	5.609232903

9.693275452	1.944695115	5.623859406
9.699575424	5.823544502	5.632709503
9.702073097	9.710083008	5.607067108
0.001403722	0.001060323	0.264396399
0.001994165	3.881085634	0.264433086
0.001968816	7.762451172	0.265141666
3.877348900	0.001283823	0.265745848
3.878720284	3.881487370	0.264147967
3.878720760	7.761273861	0.264060438
7.760569572	0.000853121	0.262310088
7.760439873	3.881053925	0.261875361
7.760780811	7.761268139	0.262151986
11.624558449	11.640566826	5.361577511
11.624709129	3.881902218	5.360574722
11.621519089	7.757256508	5.361111164
3.883294106	11.595368385	5.365554810
3.871594667	3.934543848	5.388278008
3.894294262	7.747628689	5.397442341
7.773256302	11.633890152	5.371449947
7.781994343	3.909987926	5.403401375
7.752559662	7.743330479	5.401264668
1.939564466	1.941963434	2.561661482
1.940604210	5.821379662	2.561655760
1.939992309	9.701933861	2.562861204
5.820340157	1.941529274	2.557440996
5.819457054	5.820868492	2.555202246
5.820469856	9.702482224	2.557870150
9.701293945	1.943530321	2.556173325

9.700654984	5.821850300	2.557443619
9.700472832	9.702004433	2.559784174
7.258338451	6.974469185	9.670647621
5.899278164	4.740690231	9.062799454
4.664913654	7.003130913	9.689100266
5.970375061	5.697406769	11.487663269
1.940760136	0.002769458	4.098869801
1.940165639	3.882886887	4.098313332
1.939546466	7.763078213	4.098381042
5.820614338	0.002243302	4.095010281
5.820399284	3.882557392	4.094654560
5.820059299	7.762651443	4.094202995
9.700977325	0.003473720	4.094982147
9.700627327	3.883723736	4.094614983
9.700263023	7.764190197	4.095287323
0.001347410	1.941884875	1.329203486
0.001188194	5.821822166	1.330420136
0.000927704	9.702592850	1.330575466
3.878973722	1.942084074	1.330310225
3.878939152	5.821653366	1.328689575
3.878876209	9.701571465	1.330479503
7.760471821	1.941922188	1.327139735
7.760471821	5.821761608	1.326826453
7.760714531	9.702084541	1.327475786
0.014505394	1.970054746	6.831778526
0.013107588	5.868490219	6.861155987
0.012918116	9.731803894	6.860182285
3.897530794	1.858934045	6.923213959

3.903353453 5.799028873 6.833986282

3.870040417 9.704613686 6.846562862

7.740246296 1.886386275 6.828636169

7.748097420 5.812539577 6.814670086

7.782177448 9.749215126 6.831515789

TiO2_110_Pd10

1.0

11.8360004425 0.0000000000 0.0000000000

0.0000000000 12.9938001633 0.0000000000

0.0000000000 0.0000000000 19.0447998047

O Ti Pd

96 48 10

Cartesian

2.894967318 3.248450041 19.042133331

2.894967318 9.745349884 19.042133331

5.853967667 3.248450041 19.042133331

5.853967667 9.745349884 19.042133331

8.812967300 3.248450041 19.042133331

8.812967300 9.745349884 19.042133331

11.771967888 3.248450041 19.042133331

11.771967888 9.745349884 19.042133331

2.893310308 0.000000000 3.217809439

2.893310308 6.496900082 3.217809439

5.852310658 0.000000000 3.217809439

5.852428436 6.496900082 3.217809439

8.811309814 0.000000000 3.217809439

8.811309814 6.496900082 3.217809439

11.770310402	0.000000000	3.217809439
11.770310402	6.496900082	3.217809439
2.900317192	3.146367550	6.512630939
2.933832169	9.726785660	6.517506599
5.873107433	3.086225271	6.473622799
5.885790825	9.718057632	6.523687840
8.809265137	3.104153633	6.508354187
8.813790321	9.717393875	6.556962490
11.792618752	3.155513763	6.522076607
11.776374817	9.730433464	6.533092499
2.899346590	3.248450041	2.571429014
2.899346590	9.745349884	2.571429014
5.858346939	3.248450041	2.571429014
5.858346939	9.745349884	2.571429014
8.817346573	3.248450041	2.571429014
8.817346573	9.745349884	2.571429014
11.776347160	3.248450041	2.571429014
11.776347160	9.745349884	2.571429014
2.888254404	0.007934487	5.865884781
2.877806902	6.519889832	5.788609028
5.846935749	0.003530193	5.863798141
5.818570137	6.537996769	5.856875896
8.803557396	0.001050091	5.861399651
8.830057144	6.536348820	5.854645729
11.764815331	0.008970034	5.863209248
11.777760506	6.521226883	5.784391880
2.846042871	3.225285530	9.101829529
2.828528404	9.720665932	9.119963646

5.839223385	3.284593582	9.062509537
5.807699203	9.771639824	9.109596252
8.775490761	3.289512396	9.092800140
8.806850433	9.792023659	9.137001038
11.709013939	3.221838474	9.098253250
11.719627380	9.710441589	9.120356560
1.416650891	1.208163500	1.045178652
1.416650891	7.705063820	1.045178652
4.375650883	1.208163500	1.045178652
4.375650883	7.705063820	1.045178652
7.334650993	1.208163500	1.045178652
7.334650993	7.705063820	1.045178652
10.293651581	1.208163500	1.045178652
10.293651581	7.705063820	1.045178652
1.417096734	4.552315235	4.556488514
1.417591095	11.062950134	4.551582813
4.376470566	4.548542023	4.560978889
4.386511803	11.060882568	4.544958115
7.335274696	4.550848484	4.567788124
7.339532375	11.053237915	4.545472622
10.293399811	4.548766613	4.565907955
10.287585258	11.058747292	4.552458763
1.392178893	1.168568611	8.084391594
1.391452193	7.679746628	7.976275444
4.359755993	1.164961100	8.084866524
4.275166988	7.663680553	8.098743439
7.314738274	1.163854957	8.079939842
7.318763733	7.680395126	8.008436203

10.259072304	1.161613464	8.079004288
10.336583138	7.665186882	8.079372406
1.416650891	5.288736343	1.045178652
1.416650891	11.785635948	1.045178652
4.375650883	5.288736343	1.045178652
4.375650883	11.785635948	1.045178652
7.334650993	5.288736343	1.045178652
7.334650993	11.785635948	1.045178652
10.293651581	5.288736343	1.045178652
10.293651581	11.785635948	1.045178652
1.419451833	1.930418015	4.516269207
1.421558976	8.448934555	4.524348736
4.376847744	1.928051829	4.505270004
4.375756264	8.450948715	4.522732258
7.340903759	1.923924327	4.496736050
7.339138508	8.445982933	4.535691261
10.299178123	1.929283023	4.516583443
10.302226067	8.451000214	4.533351421
1.389260292	5.238205910	7.992523670
1.391728878	11.742914200	8.006923676
4.289395332	5.189407349	7.817074299
4.344908237	11.744339943	8.016163826
7.308962345	5.178331375	7.675634861
7.308944225	11.738012314	8.000772476
10.332495689	5.186341763	7.794103622
10.281278610	11.745106697	8.005571365
2.894138813	0.000000000	1.364369512
2.894138813	6.496900082	1.364369512

5.853138924	0.000000000	1.364369512
5.853138924	6.496900082	1.364369512
8.812139511	0.000000000	1.364369512
8.812139511	6.496900082	1.364369512
11.771139145	0.000000000	1.364369512
11.771139145	6.496900082	1.364369512
2.882038355	3.319206715	4.495682240
2.892946243	9.825197220	4.495334625
5.838744164	3.309454441	4.459149361
5.851177216	9.796693802	4.456585407
8.808558464	3.301592112	4.479172230
8.797253609	9.787002563	4.467169285
11.766772270	3.316953659	4.496953487
11.754980087	9.819241524	4.496152878
2.863385677	12.959211349	7.702366352
2.850168467	6.451442719	7.628936291
5.826129913	12.954451561	7.698271275
5.817478180	6.323313236	8.078861237
8.789553642	12.939639091	7.694103241
8.796832085	6.319603443	8.065596581
11.756849289	12.963302612	7.698436260
11.759840012	6.446484089	7.622923851
1.411087990	3.248450041	1.092790604
1.411087990	9.745349884	1.092790604
4.370088100	3.248450041	1.092790604
4.370088100	9.745349884	1.092790604
7.329088211	3.248450041	1.092790604
7.329088211	9.745349884	1.092790604

10.288088799	3.248450041	1.092790604
10.288088799	9.745349884	1.092790604
1.406201601	0.080399461	4.535963058
1.406437039	6.601039886	4.466053963
4.363615990	0.078429125	4.537094593
4.436130047	6.584348679	4.574210167
7.323033810	0.071690075	4.531123161
7.318918228	6.554780006	4.727749825
10.283321381	0.073176928	4.535615921
10.206973076	6.575311661	4.574614048
1.289638996	3.204931736	7.975123405
1.268400788	9.690368652	7.985065937
4.195285320	3.173747778	7.938774109
4.182021618	9.725150108	7.958056450
7.222608089	3.148889542	7.756930828
7.205194950	9.706836700	7.823035717
10.229746819	3.164441586	7.935128212
10.209855080	9.724175453	7.931260586
5.975590706	9.265297890	11.098004341
7.302803040	7.167369843	10.159626961
8.638598442	9.263701439	11.112403870
10.104324341	7.183987141	10.254800797
8.703403473	4.903699398	10.397174835
8.692232132	6.596412659	12.441754341
7.293673515	8.695088387	13.293860435
4.513172150	7.168300152	10.276315689
5.913783073	4.884499550	10.389011383
5.968334675	6.566865444	12.437314034

TiO2_110_Pd22_1

1.0

17.7539997101	0.0000000000	0.0000000000
0.0000000000	19.4906997681	0.0000000000
0.0000000000	0.0000000000	20.1963996887

O	Ti	Pd
144	72	22

Cartesian

0.000000000	0.000000000	0.000000000
0.000000000	6.496835232	0.000000000
0.000000000	12.993865013	0.000000000
2.959059000	0.000000000	0.000000000
2.959059000	6.496835232	0.000000000
2.959059000	12.993865013	0.000000000
5.917940617	0.000000000	0.000000000
5.917940617	6.496835232	0.000000000
5.917940617	12.993865013	0.000000000
8.876999855	0.000000000	0.000000000
8.876999855	6.496835232	0.000000000
8.876999855	12.993865013	0.000000000
11.836059570	0.000000000	0.000000000
11.836059570	6.496835232	0.000000000
11.836059570	12.993865013	0.000000000
14.794939995	0.000000000	0.000000000
14.794939995	6.496835232	0.000000000
14.794939995	12.993865013	0.000000000
17.753608704	3.241810083	3.147770405

0.000177540	9.753301620	3.151224136
0.000124278	16.242029190	3.138742685
2.950306416	3.221383810	3.147467613
2.961882114	9.751392365	3.154879808
2.958526373	16.240684509	3.138419628
5.911407471	3.188483477	3.145467997
5.906329632	9.763865471	3.152415514
5.918171406	16.240665436	3.138520479
8.877727509	3.173963070	3.138015747
8.877887726	9.781602859	3.145690203
8.876609802	16.240293503	3.139894009
11.842024803	3.190393686	3.147406816
11.849090576	9.762287140	3.154314280
11.835651398	16.241678238	3.138823509
14.802326202	3.222124577	3.147629261
14.790874481	9.749111176	3.155970335
14.795188904	16.240879059	3.138702154
0.000000000	0.000000000	2.547977686
0.000000000	6.496835232	2.547977686
0.000000000	12.993865013	2.547977686
2.959059000	0.000000000	2.547977686
2.959059000	6.496835232	2.547977686
2.959059000	12.993865013	2.547977686
5.917940617	0.000000000	2.547977686
5.917940617	6.496835232	2.547977686
5.917940617	12.993865013	2.547977686
8.876999855	0.000000000	2.547977686
8.876999855	6.496835232	2.547977686

8.876999855	12.993865013	2.547977686
11.836059570	0.000000000	2.547977686
11.836059570	6.496835232	2.547977686
11.836059570	12.993865013	2.547977686
14.794939995	0.000000000	2.547977686
14.794939995	6.496835232	2.547977686
14.794939995	12.993865013	2.547977686
17.751495361	3.222943306	5.752601624
0.001136256	9.762540817	5.757448673
17.752916336	16.245498657	5.736746788
2.946595907	3.232902765	5.746905804
2.944678307	9.771584511	5.754863262
2.957869530	16.243412018	5.736726761
5.907536983	3.316108704	5.773302555
5.905566216	9.797662735	5.759346962
5.917514801	16.246297836	5.736423492
8.872809410	3.308117390	5.711461067
8.880284309	9.789652824	5.726042747
8.876307487	16.245536804	5.737190723
11.840178490	3.313029289	5.774190903
11.851770401	9.782831192	5.764678478
11.835420609	16.246297836	5.736060143
14.801456451	3.229141235	5.747875214
14.811841965	9.771135330	5.755751610
14.794425964	16.243705750	5.736646175
1.479440808	4.522427082	1.273988843
1.479440808	11.019262314	1.273988843
1.479440808	17.516292572	1.273988843

4.438499928	4.522427082	1.273988843
4.438499928	11.019262314	1.273988843
4.438499928	17.516292572	1.273988843
7.397559166	4.522427082	1.273988843
7.397559166	11.019262314	1.273988843
7.397559166	17.516292572	1.273988843
10.356440544	4.522427082	1.273988843
10.356440544	11.019262314	1.273988843
10.356440544	17.516292572	1.273988843
13.315500259	4.522427082	1.273988843
13.315500259	11.019262314	1.273988843
13.315500259	17.516292572	1.273988843
16.274559021	4.522427082	1.273988843
16.274559021	11.019262314	1.273988843
16.274559021	17.516292572	1.273988843
1.476085305	1.218051791	4.689603806
1.457940698	7.730401516	4.693078041
1.477470040	14.222109795	4.689382076
4.444003582	1.216921329	4.711295128
4.367661476	7.728588581	4.731874943
4.436404705	14.223688126	4.686696053
7.393457890	1.213861346	4.729633331
7.373094082	7.760612011	4.570122242
7.397150517	14.221758842	4.689422131
10.358251572	1.215186596	4.729996681
10.380728722	7.760046482	4.569374561
10.358304977	14.220901489	4.689725399
13.306142807	1.215284109	4.711617947

13.385219574	7.722858429	4.744134426
13.317771912	14.221993446	4.687523842
16.274665833	1.217428088	4.690189362
16.293964386	7.730499268	4.692956448
16.275091171	14.220960617	4.689280510
1.479440808	1.974407911	1.273988843
1.479440808	8.471437454	1.273988843
1.479440808	14.968273163	1.273988843
4.438499928	1.974407911	1.273988843
4.438499928	8.471437454	1.273988843
4.438499928	14.968273163	1.273988843
7.397559166	1.974407911	1.273988843
7.397559166	8.471437454	1.273988843
7.397559166	14.968273163	1.273988843
10.356440544	1.974407911	1.273988843
10.356440544	8.471437454	1.273988843
10.356440544	14.968273163	1.273988843
13.315500259	1.974407911	1.273988843
13.315500259	8.471437454	1.273988843
13.315500259	14.968273163	1.273988843
16.274559021	1.974407911	1.273988843
16.274559021	8.471437454	1.273988843
16.274559021	14.968273163	1.273988843
1.455224276	5.260871410	4.705357075
1.477239251	11.772246361	4.682515144
1.482068300	18.263467789	4.684635639
4.381260872	5.217582226	4.573272705
4.431966305	11.777508736	4.691522598

4.436866760	18.261577606	4.682555199
7.382202148	5.193861961	4.460899830
7.393706322	11.778406143	4.678233624
7.400453091	18.262376785	4.682979584
10.371691704	5.194583416	4.464777470
10.362868309	11.776943207	4.678677559
10.351256371	18.262065887	4.682838440
13.371230125	5.218517780	4.582441807
13.322245598	11.773824692	4.692552567
13.314612389	18.260915756	4.682010174
16.296483994	5.260364532	4.705862045
16.276903152	11.770765305	4.682979584
16.269853592	18.262706757	4.683504581
0.000000000	3.248514891	1.273988843
0.000000000	9.745349884	1.273988843
0.000000000	16.242183685	1.273988843
2.959059000	3.248514891	1.273988843
2.959059000	9.745349884	1.273988843
2.959059000	16.242183685	1.273988843
5.917940617	3.248514891	1.273988843
5.917940617	9.745349884	1.273988843
5.917940617	16.242183685	1.273988843
8.876999855	3.248514891	1.273988843
8.876999855	9.745349884	1.273988843
8.876999855	16.242183685	1.273988843
11.836059570	3.248514891	1.273988843
11.836059570	9.745349884	1.273988843
11.836059570	16.242183685	1.273988843

14.794939995	3.248514891	1.273988843
14.794939995	9.745349884	1.273988843
14.794939995	16.242183685	1.273988843
17.752792358	19.486061096	4.362684727
17.753253937	6.502701759	4.364159107
17.753839493	12.991953850	4.362402439
2.954904795	0.002046523	4.363189697
2.932818651	6.476077080	4.365270138
2.954620600	12.996905327	4.362624168
5.912490368	19.477251053	4.362220287
5.922255039	6.426239967	4.444177151
5.915810108	12.996905327	4.363331318
8.876715660	19.481033325	4.363351345
8.874425888	6.438460350	4.427010536
8.877851486	12.991662979	4.361715317
11.839059830	19.476665497	4.362583637
11.826932907	6.432729721	4.442157745
11.839237213	12.994625092	4.362906933
14.796432495	19.490446091	4.362563610
14.819245338	6.475336552	4.363593578
14.798491478	12.994585991	4.363997459
1.479440808	0.000000000	1.273988843
1.479440808	6.496835232	1.273988843
1.479440808	12.993865013	1.273988843
4.438499928	0.000000000	1.273988843
4.438499928	6.496835232	1.273988843
4.438499928	12.993865013	1.273988843
7.397559166	0.000000000	1.273988843

7.397559166	6.496835232	1.273988843
7.397559166	12.993865013	1.273988843
10.356440544	0.000000000	1.273988843
10.356440544	6.496835232	1.273988843
10.356440544	12.993865013	1.273988843
13.315500259	0.000000000	1.273988843
13.315500259	6.496835232	1.273988843
13.315500259	12.993865013	1.273988843
16.274559021	0.000000000	1.273988843
16.274559021	6.496835232	1.273988843
16.274559021	12.993865013	1.273988843
1.462769866	3.247072458	4.663934231
1.465361953	9.739327431	4.665893078
1.477789640	16.240879059	4.658824444
4.396955490	3.236898422	4.642950535
4.390599728	9.753926277	4.641031742
4.436032295	16.238403320	4.658077240
7.374514580	3.219122887	4.585249424
7.375206470	9.748761177	4.579977989
7.396653652	16.235227585	4.658501625
10.370342255	3.221325159	4.587289333
10.387244225	9.746753693	4.582179070
10.355197906	16.234212875	4.658481121
13.345823288	3.236527920	4.644949913
13.366293907	9.746772766	4.645212173
13.315535545	16.237234116	4.657673359
16.280719757	3.245143175	4.664741993
16.290697098	9.738293648	4.665429115

16.273937225	16.239515305	4.658723831
8.894008636	9.336239815	7.766263008
11.560801506	4.608946323	7.514898300
8.855570793	6.789994717	9.113181114
6.119892120	4.682192326	7.481958389
11.550344467	9.119814873	7.782218456
6.237104416	9.187311172	7.785227299
11.593432426	6.712810993	9.193784714
8.840479851	4.671141148	7.457116604
8.881935120	8.861154556	12.333759308
6.117069244	6.781145573	9.178859711
12.923847198	6.905477047	6.876894474
10.274506569	8.952331543	10.079841614
7.543656826	7.023395538	6.756886959
10.115678787	2.500520229	8.511974335
10.177941322	6.661901474	11.520672798
7.500478745	4.588305950	10.053848267
10.194293022	6.985876083	6.759512424
7.499875069	8.989734650	10.075862885
4.810890198	7.006087780	6.859464645
10.155483246	4.542346478	10.051162720
7.493448734	2.549344540	8.514479637
7.514913082	6.703494549	11.525601387

TiO2_110_Pd22_2

1.0

17.7539997101	0.0000000000	0.0000000000
0.0000000000	19.4906997681	0.0000000000

0.0000000000 0.0000000000 20.1963996887

O Ti Pd

144 72 22

Cartesian

0.000000000	0.000000000	0.000000000
0.000000000	6.496835232	0.000000000
0.000000000	12.993865013	0.000000000
2.959059000	0.000000000	0.000000000
2.959059000	6.496835232	0.000000000
2.959059000	12.993865013	0.000000000
5.917940617	0.000000000	0.000000000
5.917940617	6.496835232	0.000000000
5.917940617	12.993865013	0.000000000
8.876999855	0.000000000	0.000000000
8.876999855	6.496835232	0.000000000
8.876999855	12.993865013	0.000000000
11.836059570	0.000000000	0.000000000
11.836059570	6.496835232	0.000000000
11.836059570	12.993865013	0.000000000
14.794939995	0.000000000	0.000000000
14.794939995	6.496835232	0.000000000
14.794939995	12.993865013	0.000000000
17.753129959	3.248261452	3.149588108
17.746648788	9.746753693	3.155808687
17.753414154	16.242534637	3.137450218
2.958278179	3.240036488	3.150517225
2.955224276	9.751469612	3.150496960
2.956165314	16.240314484	3.137914658

5.909862995	3.221383810	3.153910160
5.908584595	9.769440651	3.153284073
5.915525913	16.243900299	3.137975454
8.864997864	3.212320566	3.131774902
8.856565475	9.788560867	3.129876375
8.878011703	16.240371704	3.138823509
11.850244522	3.216336012	3.141489267
11.845451355	9.780744553	3.137308836
11.835260391	16.243822098	3.138783216
14.797284126	3.229570150	3.155041218
14.802237511	9.774761200	3.163099527
14.795188904	16.240392685	3.137167215
0.000000000	0.000000000	2.547977686
0.000000000	6.496835232	2.547977686
0.000000000	12.993865013	2.547977686
2.959059000	0.000000000	2.547977686
2.959059000	6.496835232	2.547977686
2.959059000	12.993865013	2.547977686
5.917940617	0.000000000	2.547977686
5.917940617	6.496835232	2.547977686
5.917940617	12.993865013	2.547977686
8.876999855	0.000000000	2.547977686
8.876999855	6.496835232	2.547977686
8.876999855	12.993865013	2.547977686
11.836059570	0.000000000	2.547977686
11.836059570	6.496835232	2.547977686
11.836059570	12.993865013	2.547977686
14.794939995	0.000000000	2.547977686

14.794939995	6.496835232	2.547977686
14.794939995	12.993865013	2.547977686
0.000124278	3.238827944	5.754842758
17.745300293	9.756011009	5.762032509
17.751230240	16.243158340	5.735393524
2.945139885	3.234968901	5.751348972
2.934434175	9.756850243	5.751530647
2.954442978	16.240547180	5.735877991
5.886924267	3.248300552	5.790307999
5.876307964	9.776165009	5.785379410
5.914425373	16.245166779	5.736161232
8.882734299	3.155076265	5.681893349
8.868673325	9.802379608	5.690295219
8.874709129	16.241092682	5.737655640
11.838242531	3.246156454	5.736524582
11.821873665	9.809045792	5.711238861
11.835633278	16.245439529	5.736868382
14.801260948	3.273774862	5.768233299
14.780701637	9.664522171	5.805596352
14.794301033	16.240041733	5.735171795
1.479440808	4.522427082	1.273988843
1.479440808	11.019262314	1.273988843
1.479440808	17.516292572	1.273988843
4.438499928	4.522427082	1.273988843
4.438499928	11.019262314	1.273988843
4.438499928	17.516292572	1.273988843
7.397559166	4.522427082	1.273988843
7.397559166	11.019262314	1.273988843

7.397559166	17.516292572	1.273988843
10.356440544	4.522427082	1.273988843
10.356440544	11.019262314	1.273988843
10.356440544	17.516292572	1.273988843
13.315500259	4.522427082	1.273988843
13.315500259	11.019262314	1.273988843
13.315500259	17.516292572	1.273988843
16.274559021	4.522427082	1.273988843
16.274559021	11.019262314	1.273988843
16.274559021	17.516292572	1.273988843
1.475037813	1.226140380	4.685382843
1.472765207	7.726366520	4.696046829
1.468823910	14.215756416	4.689664841
4.435339928	1.220975399	4.694390774
4.413448811	7.731492996	4.687826633
4.428557873	14.222207069	4.685585022
7.379112720	1.217096686	4.693683624
7.364553928	7.761137962	4.596720695
7.388256073	14.227645874	4.681687355
10.367465973	1.217135787	4.675547123
10.331354141	7.775717258	4.551319122
10.358997345	14.223397255	4.689321518
13.319689751	1.222846508	4.704145432
13.345503807	7.757824898	4.582340717
13.313707352	14.221740723	4.683969021
16.273315430	1.228128433	4.694269180
16.296627045	7.728705883	4.689321518
16.276140213	14.219108582	4.684231758

1.479440808	1.974407911	1.273988843
1.479440808	8.471437454	1.273988843
1.479440808	14.968273163	1.273988843
4.438499928	1.974407911	1.273988843
4.438499928	8.471437454	1.273988843
4.438499928	14.968273163	1.273988843
7.397559166	1.974407911	1.273988843
7.397559166	8.471437454	1.273988843
7.397559166	14.968273163	1.273988843
10.356440544	1.974407911	1.273988843
10.356440544	8.471437454	1.273988843
10.356440544	14.968273163	1.273988843
13.315500259	1.974407911	1.273988843
13.315500259	8.471437454	1.273988843
13.315500259	14.968273163	1.273988843
16.274559021	1.974407911	1.273988843
16.274559021	8.471437454	1.273988843
16.274559021	14.968273163	1.273988843
1.477949500	5.266191959	4.695016384
1.471771002	11.764780998	4.684635639
1.475730300	18.265514374	4.686837196
4.410803795	5.259389400	4.680676937
4.427279472	11.772987366	4.691219807
4.429338932	18.261907578	4.685605049
7.373484612	5.231693745	4.584622860
7.385095596	11.782421112	4.700590611
7.399192333	18.262279510	4.681747437
10.337302208	5.226275444	4.564022541

10.347617149	11.782225609	4.672295570
10.352446556	18.264617920	4.688149929
13.360914230	5.250502586	4.647130966
13.327572823	11.771661758	4.701661110
13.320773125	18.262454987	4.683444023
16.290822983	5.267088413	4.689563751
16.262556076	11.763280869	4.713152885
16.273723602	18.265436172	4.685403347
0.000000000	3.248514891	1.273988843
0.000000000	9.745349884	1.273988843
0.000000000	16.242183685	1.273988843
2.959059000	3.248514891	1.273988843
2.959059000	9.745349884	1.273988843
2.959059000	16.242183685	1.273988843
5.917940617	3.248514891	1.273988843
5.917940617	9.745349884	1.273988843
5.917940617	16.242183685	1.273988843
8.876999855	3.248514891	1.273988843
8.876999855	9.745349884	1.273988843
8.876999855	16.242183685	1.273988843
11.836059570	3.248514891	1.273988843
11.836059570	9.745349884	1.273988843
11.836059570	16.242183685	1.273988843
14.794939995	3.248514891	1.273988843
14.794939995	9.745349884	1.273988843
14.794939995	16.242183685	1.273988843
17.751852036	0.001754163	4.364340782
17.751443863	6.489545345	4.362483025

17.750112534	12.987335205	4.365411282
2.954230070	0.000350833	4.363977432
2.959041357	6.501162052	4.362826347
2.951602459	12.992052078	4.363512993
5.911549091	19.479084015	4.361836433
5.917336941	6.482879639	4.398715019
5.908033848	12.999108315	4.362280846
8.876094818	0.006802254	4.361230850
8.872774124	6.518196583	4.420628071
8.872330666	13.007664680	4.361614227
11.837639809	19.482181549	4.362422466
11.832578659	6.485589027	4.504766464
11.834904671	12.991292000	4.362806320
14.798455238	0.000389814	4.364260197
14.787004471	6.513850212	4.365431786
14.794852257	13.001504898	4.364058018
1.479440808	0.000000000	1.273988843
1.479440808	6.496835232	1.273988843
1.479440808	12.993865013	1.273988843
4.438499928	0.000000000	1.273988843
4.438499928	6.496835232	1.273988843
4.438499928	12.993865013	1.273988843
7.397559166	0.000000000	1.273988843
7.397559166	6.496835232	1.273988843
7.397559166	12.993865013	1.273988843
10.356440544	0.000000000	1.273988843
10.356440544	6.496835232	1.273988843
10.356440544	12.993865013	1.273988843

13.315500259	0.000000000	1.273988843
13.315500259	6.496835232	1.273988843
13.315500259	12.993865013	1.273988843
16.274559021	0.000000000	1.273988843
16.274559021	6.496835232	1.273988843
16.274559021	12.993865013	1.273988843
1.465060115	3.255239248	4.662823677
1.451105475	9.735000610	4.662278175
1.476085305	16.241035461	4.658481121
4.393032074	3.245825052	4.654058456
4.381172180	9.738918304	4.653755188
4.434434414	16.240800858	4.659047127
7.358731270	3.246780396	4.602759361
7.340320110	9.756615639	4.596155643
7.394771576	16.245166779	4.658501625
10.370466232	3.250093699	4.544472694
10.345628738	9.751021385	4.531688213
10.354328156	16.244035721	4.659794331
13.356990814	3.241245031	4.634790897
13.339840889	9.748624802	4.624510765
13.313689232	16.241678238	4.658441067
16.286880493	3.260053396	4.669367313
16.271505356	9.737865448	4.683484554
16.272552490	16.243236542	4.657612801
6.736258030	6.643814564	7.509243488
11.390628815	9.475715637	7.716115475
9.994685173	6.701955318	9.509859085
11.487778664	4.031865597	7.644438267

6.556765079	9.265430450	7.732575417
6.626857758	4.015025616	7.634380341
9.866909027	9.379548073	9.933699608
11.539922714	6.754658222	7.118200779
8.518919945	6.601149082	11.832344055
9.974197388	4.054182529	9.915362358
8.929267883	10.585710526	7.817562103
7.607571125	8.055331230	9.787922859
9.113625526	5.439016342	7.250346184
13.778488159	8.201998711	7.564177990
10.795460701	8.001653671	11.926923752
12.389308929	5.453614712	9.766675949
9.063949585	8.024028778	7.365142345
7.651388168	5.238944054	9.698533058
9.054823875	2.886689425	7.802818298
12.336367607	8.037165642	9.775401115
13.801391602	5.445682049	7.559895992
10.907738686	5.400444031	11.939626694