Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information for "The influence of oxygen vacancy and Ce^{3+} ion positions on the properties of small gold clusters supported on CeO_{2-X}(111)"

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1. Structures of Au clusters on CeO_{2-X}

Table S 1: Structures of Au_n/CeO_{2-X}

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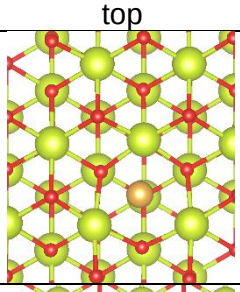
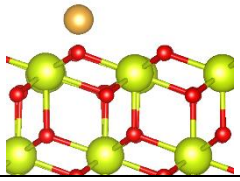
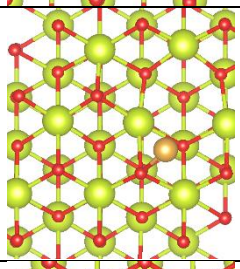
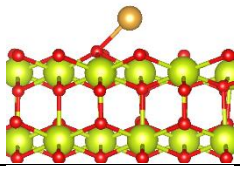
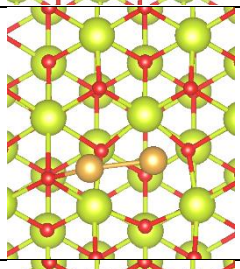
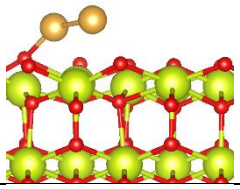
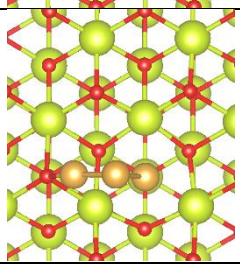
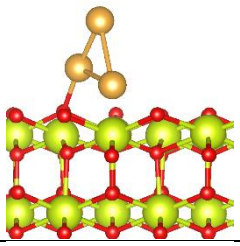
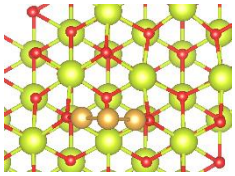
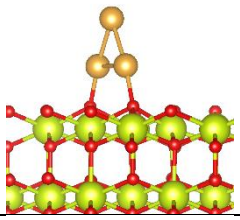
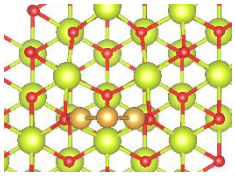
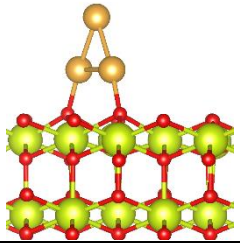
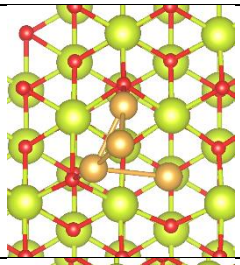
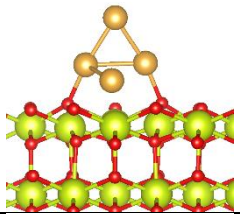
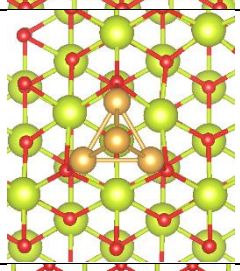
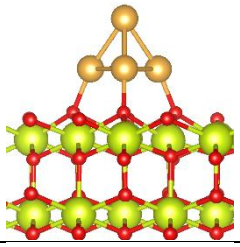
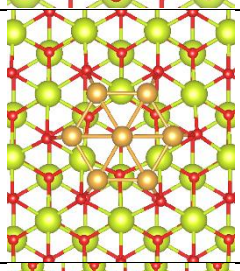
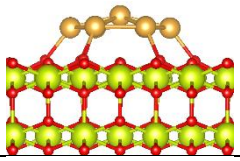
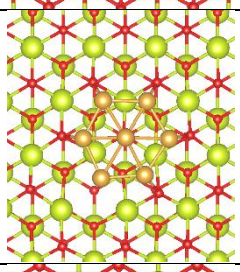
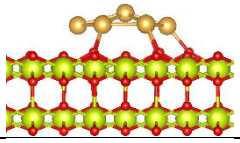
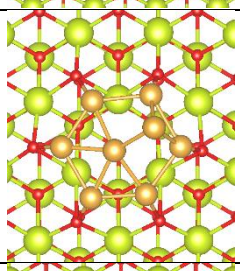
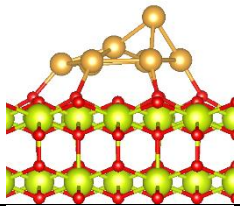
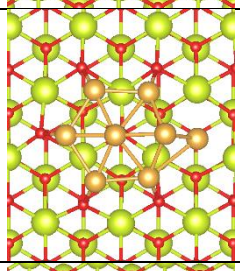
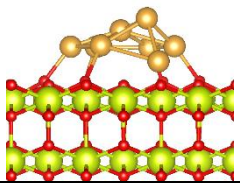
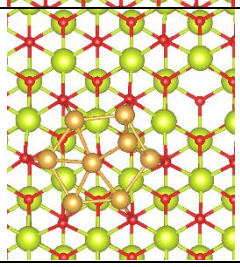
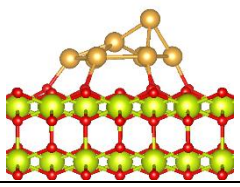
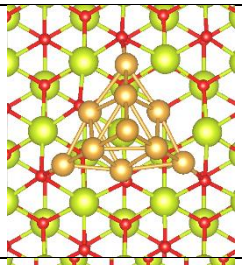
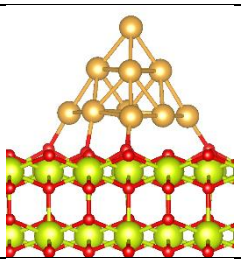
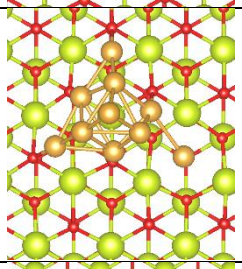
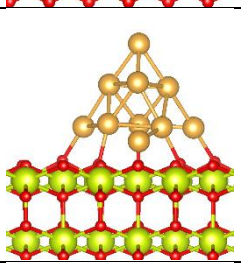
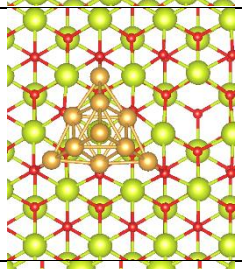
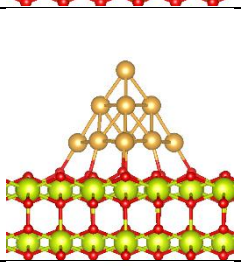
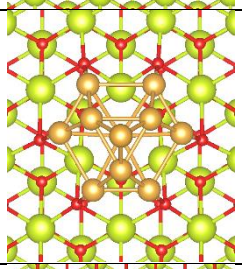
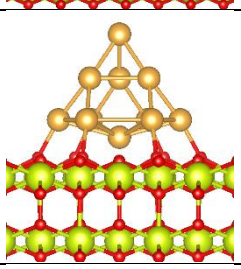
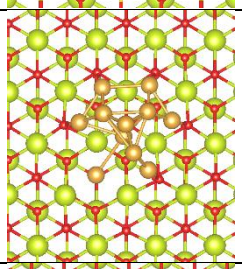
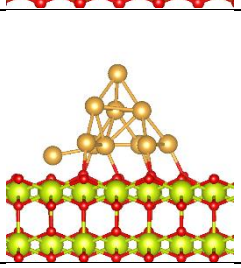
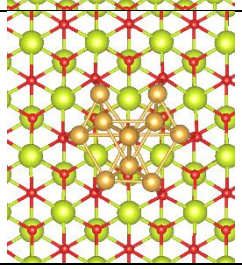
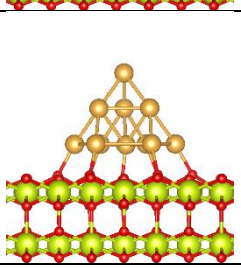
1	1			under
2	1			next
3	2			next
4	3			under/corner
5	3			next (a)
6	3			next (b)

7	4			under/corner
8	4			next
9	7			under/centre
10	7			under/corner
11	8			under/centre
12	8			under/corner
13	8			next

14	10			under/edge
15	10			under/corner
16	10			next
17	11			under/centre
18	11			under/corner
19	11			next

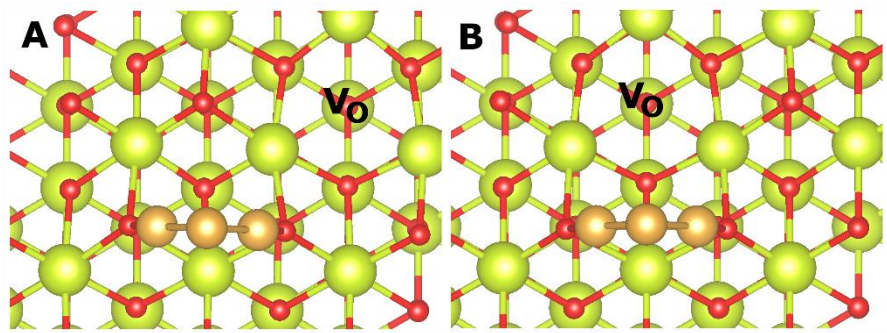


Figure S 1: Vacancy positions next to the Au cluster of Au_3/CeO_{2-x}.

2. DOS and COHP plots

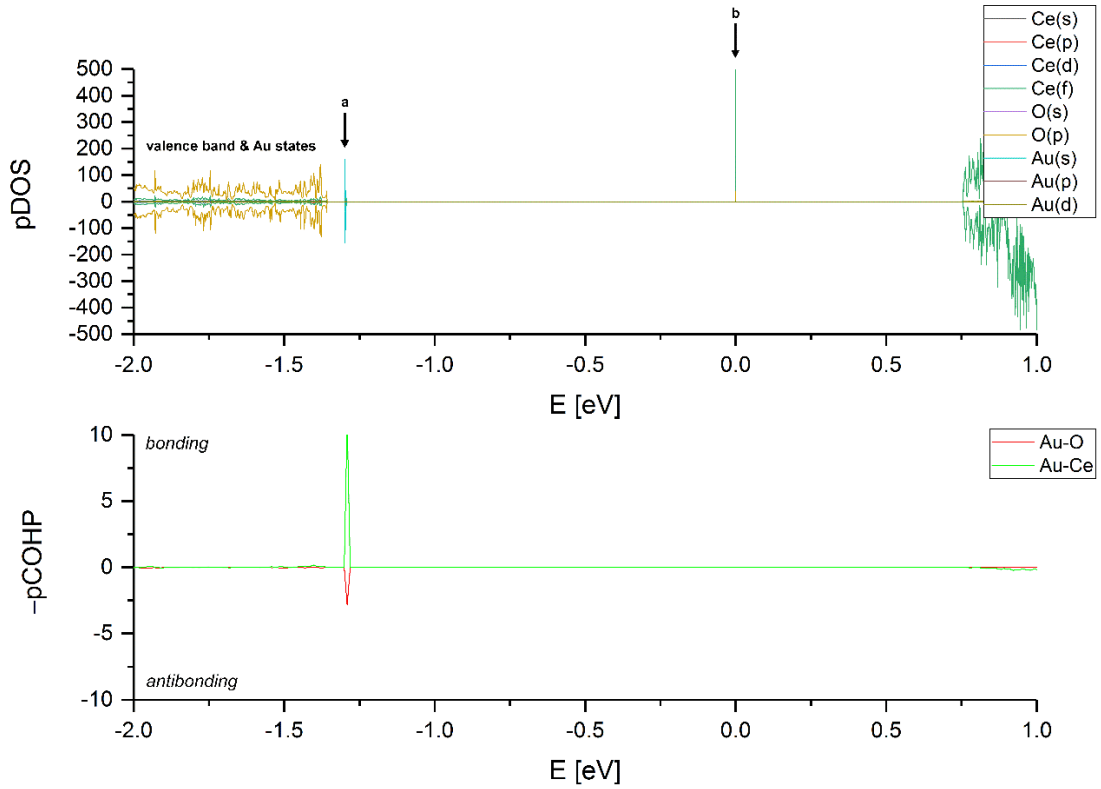


Figure S 2: DOS (top) and COHP (bottom) of Au_1/CeO_{2-x}; localisation of Ce^{3+} in 2_1 position; average COHP of all respective pairs within 4.0 Å.

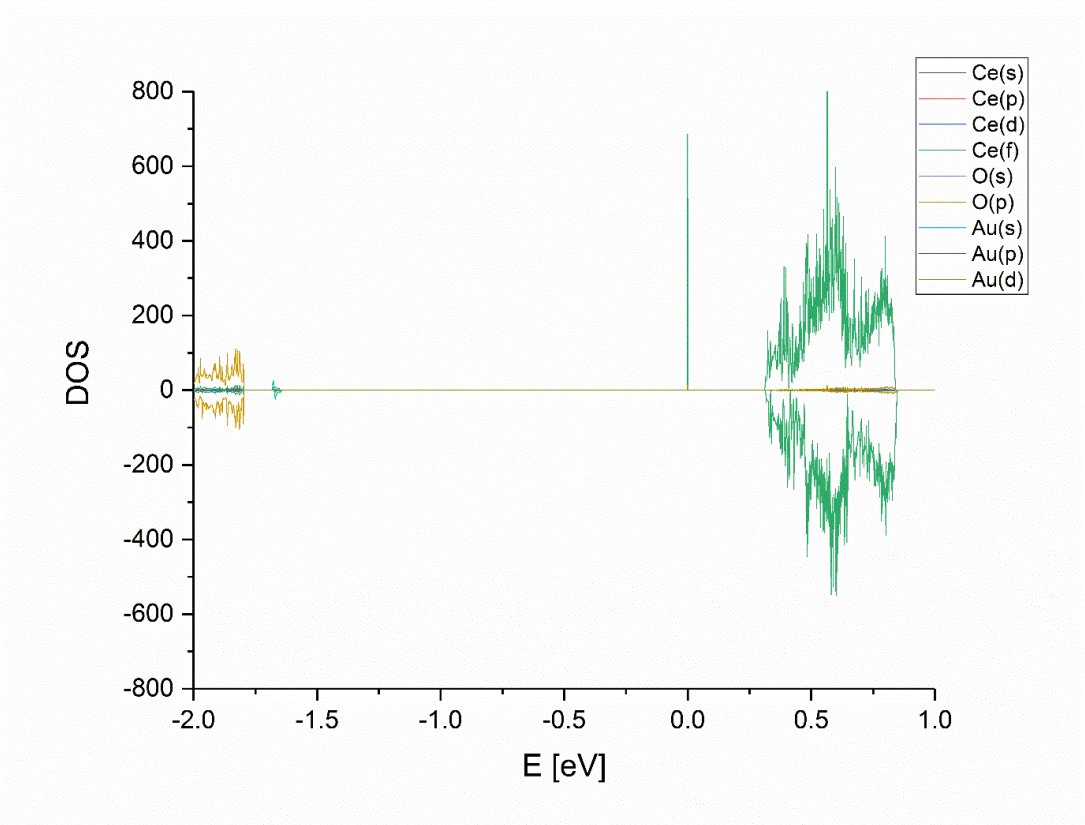


Figure S 3: DOS of Au_1/CeO_{2-x}; localisation of Ce^{3+} in 1_1 position

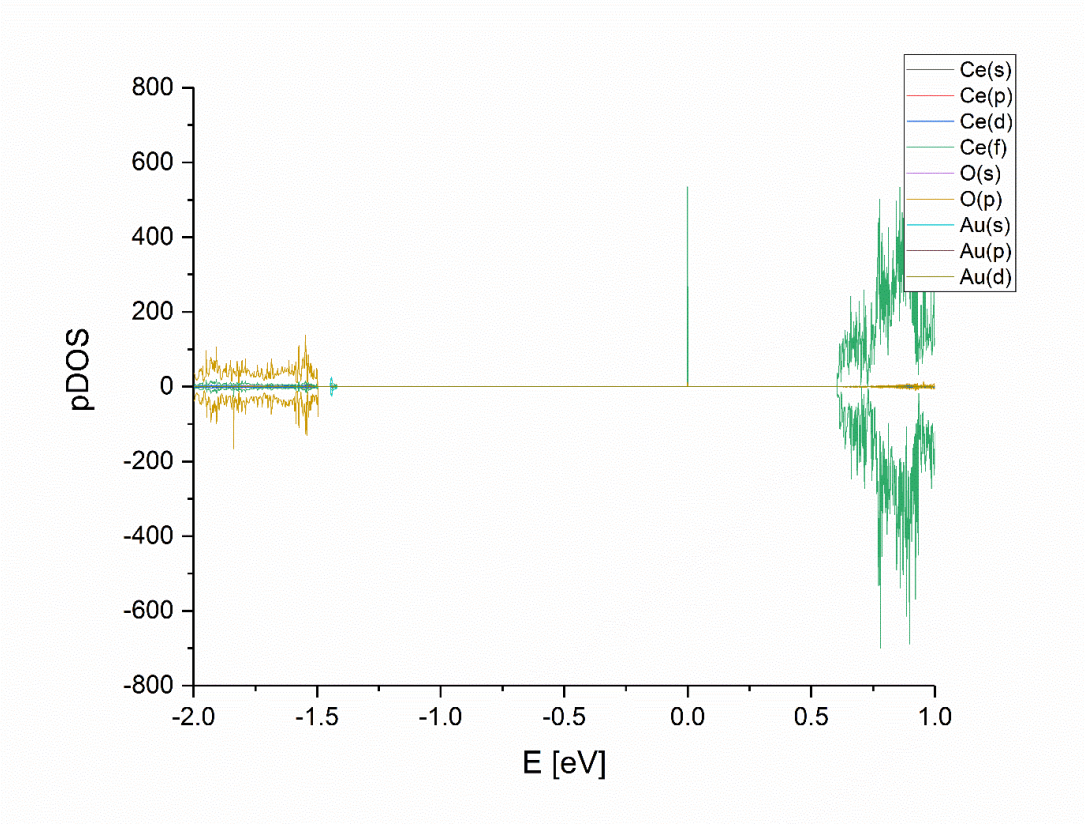


Figure S 4: DOS of Au_1/CeO_{2-x}; localisation of Ce^{3+} in 3_1 position.

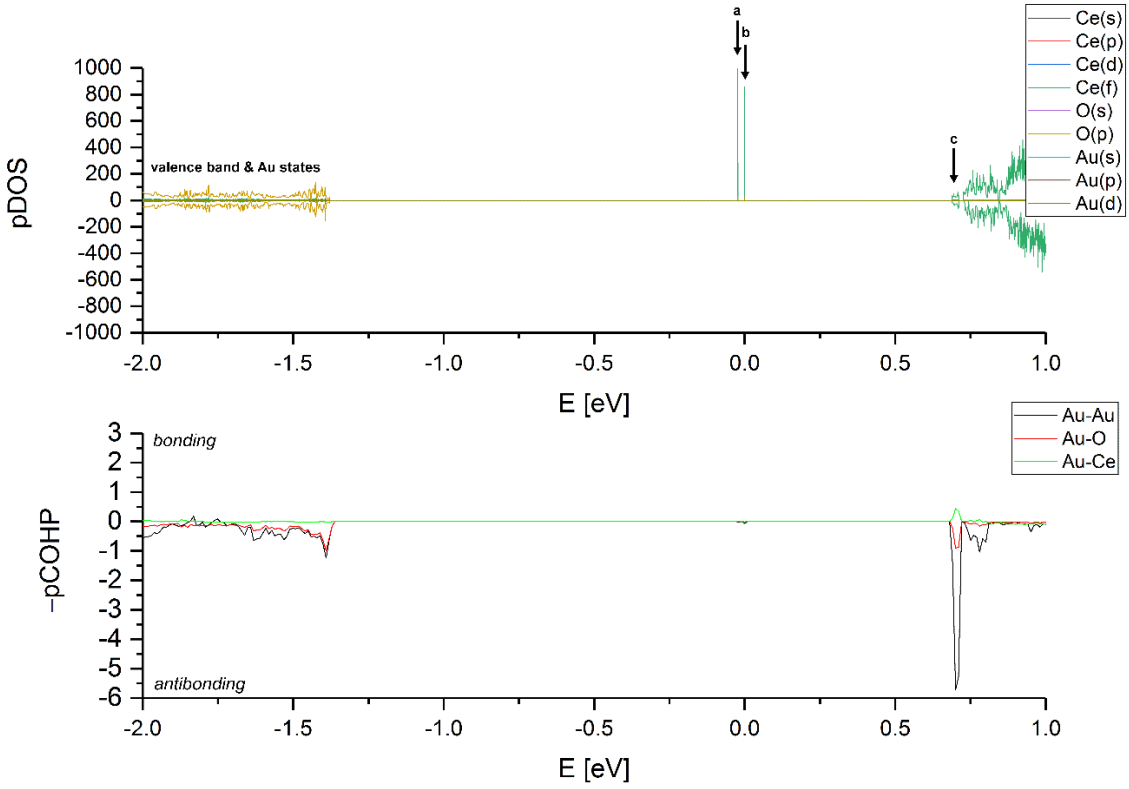


Figure S 5: DOS (top) and COHP (bottom) of Au_2/CeO_{2-x}; average COHP of all respective pairs within 4.0 Å.

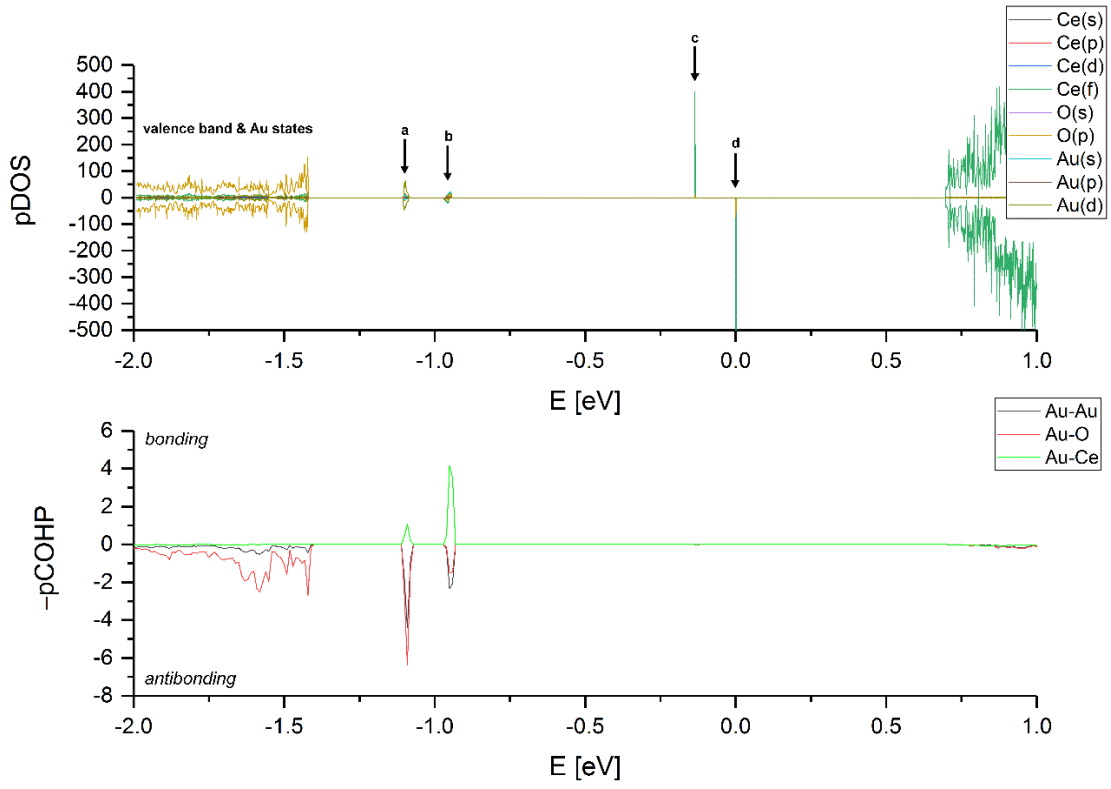


Figure S 6: DOS (top) and COHP (bottom) plot of Au_4/CeO_{2-x}; vacancy under Au_4; average COHP of all respective pairs within 4.0 Å.

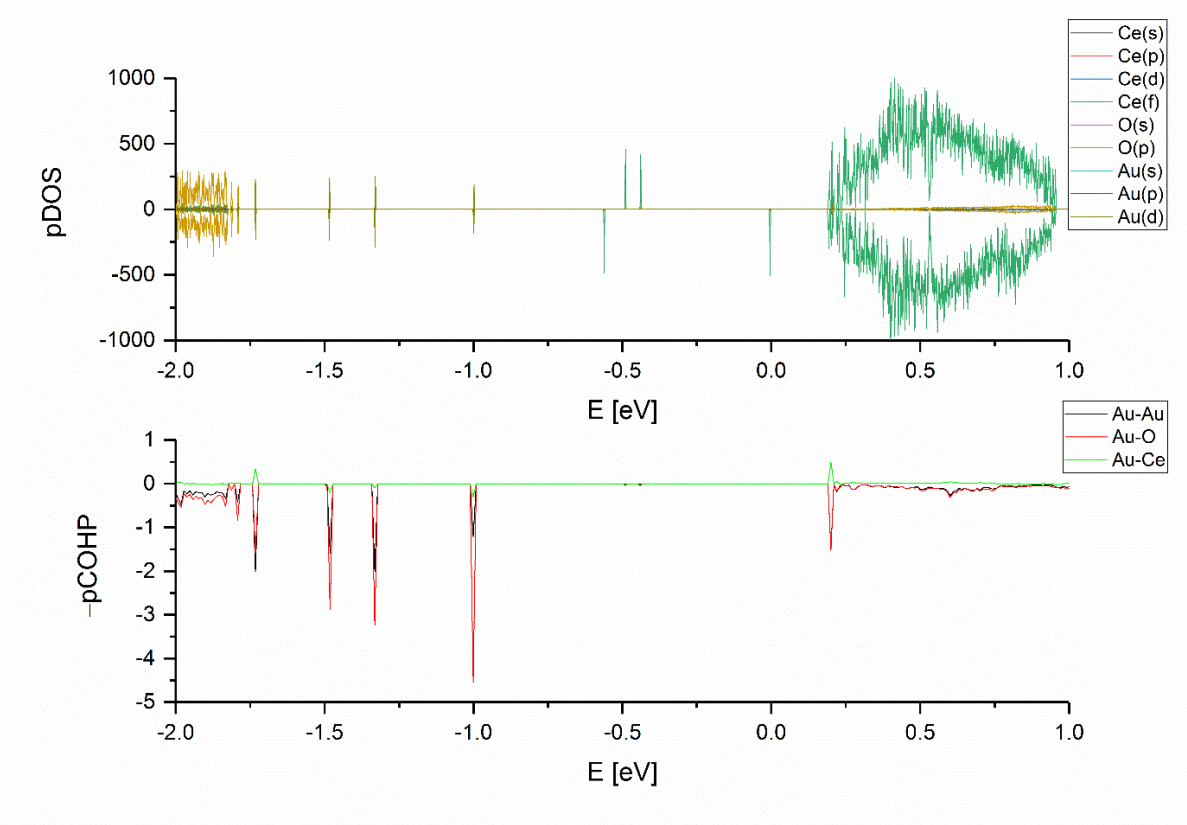


Figure S 7: DOS (top) and COHP (bottom) plot of Au_8/CeO_{2-x}; average COHP of all respective pairs with a maximum distance of 4.0 Å; vacancy under central Au atom.

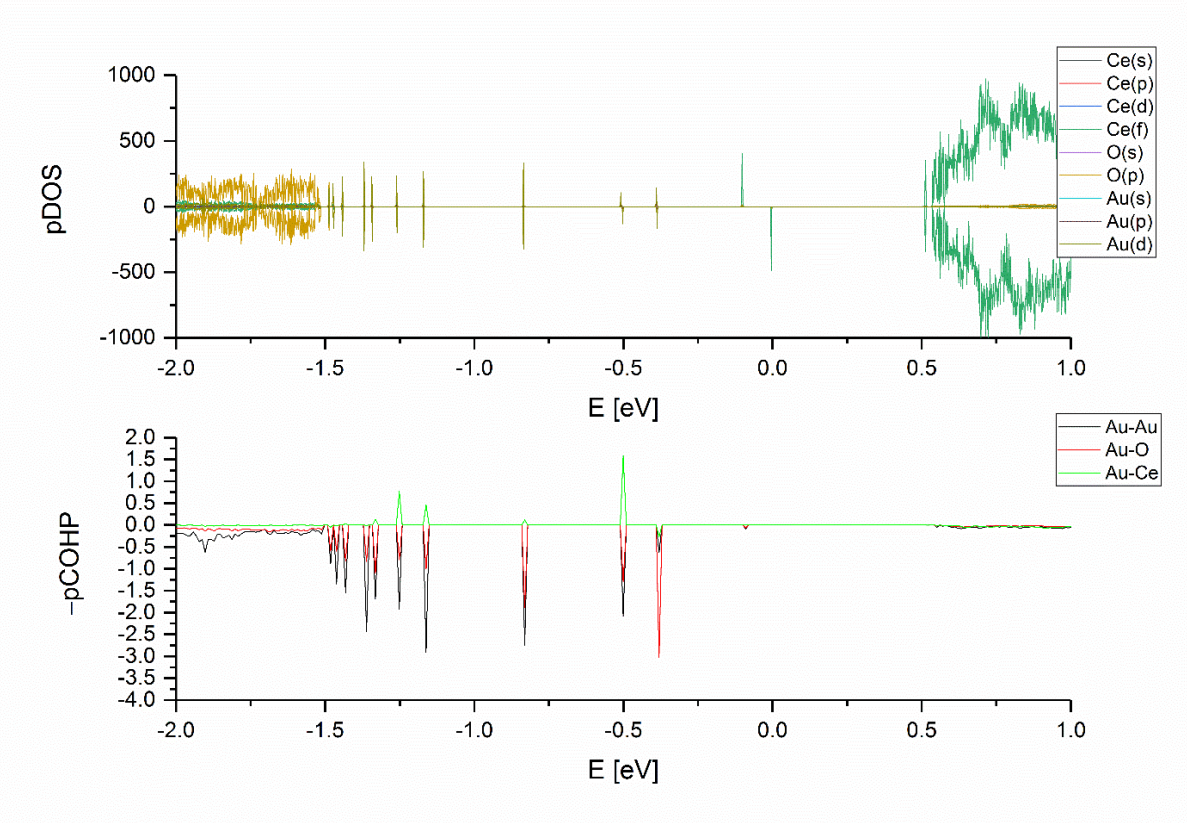


Figure S 8: DOS (top) and COHP (bottom) plot of Au_8/CeO_{2-x}; average COHP of all respective pairs with a maximum distance of 4.0 Å; vacancy under corner Au atom.

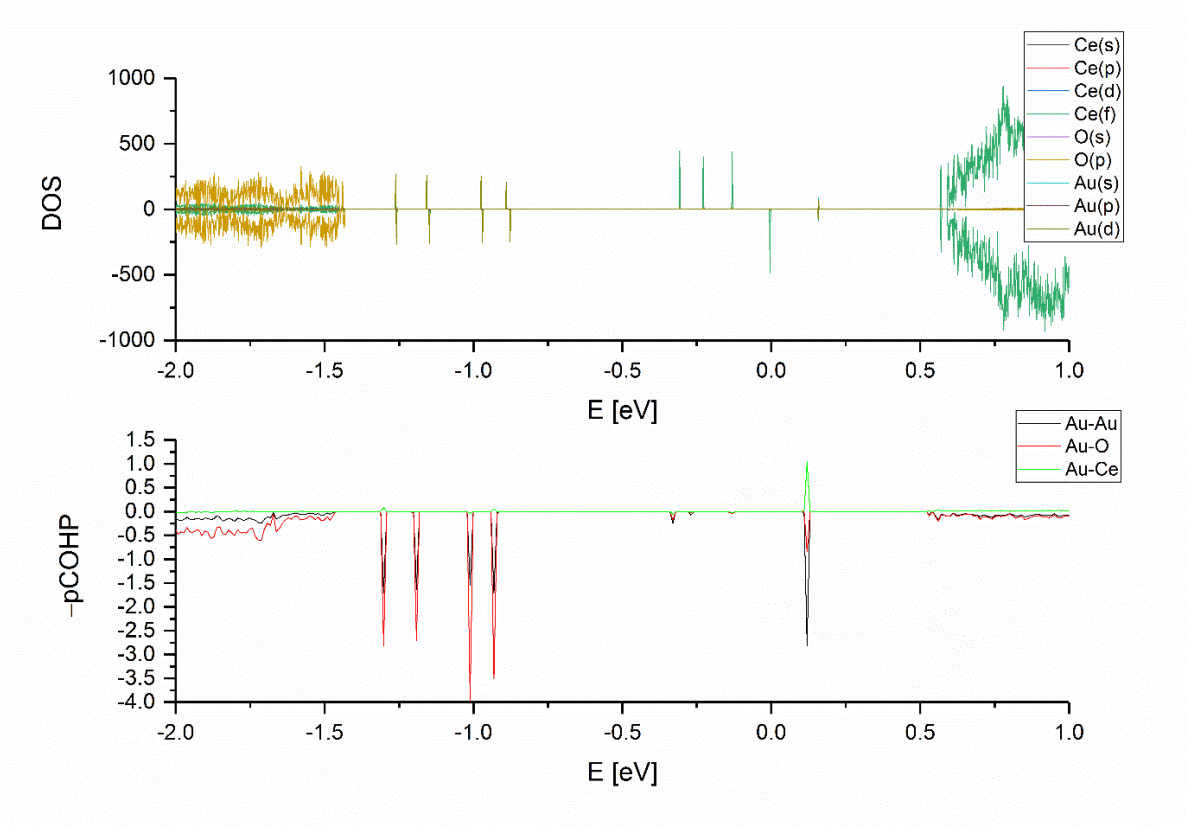


Figure S 9: DOS (top) and COHP (bottom) plot of Au_{10}/CeO_{2-x}; vacancy under edge Au atom; average COHP of all respective pairs with a maximum distance of 4.0 Å.

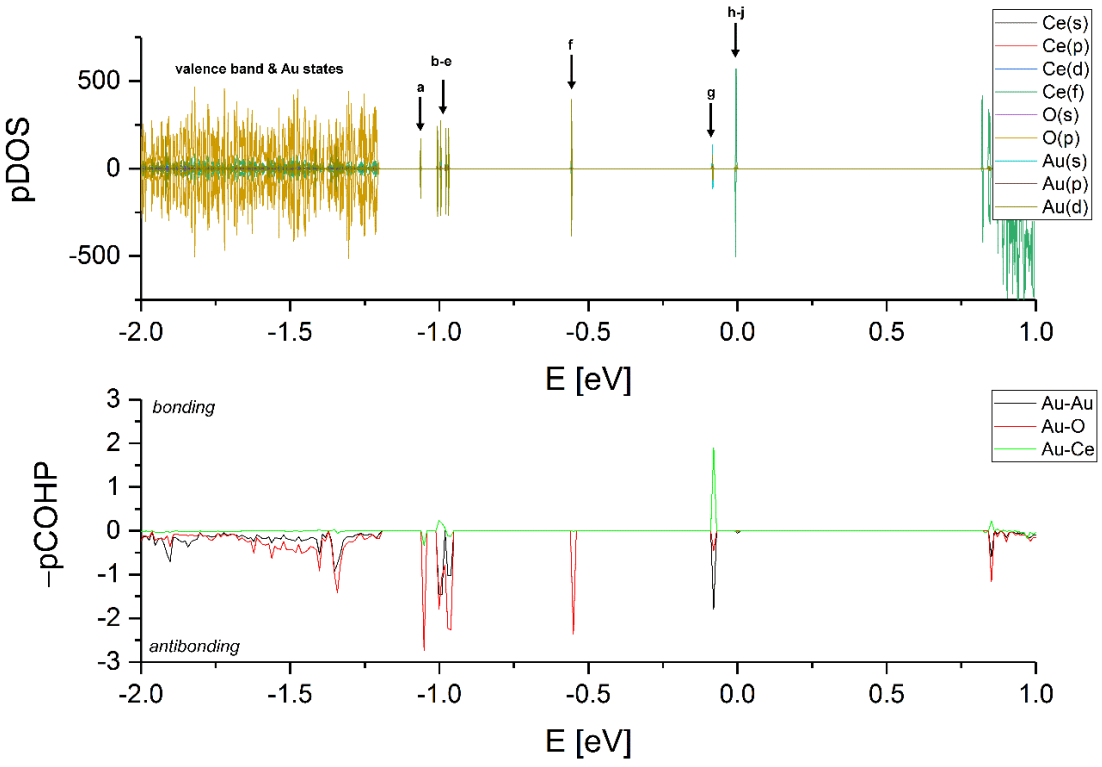


Figure S 10: DOS (top) and COHP (bottom) plot of Au_{11}/CeO_{2-x}; average COHP of all respective pairs with a maximum distance of 4.0 Å.

2. Iso-surfaces

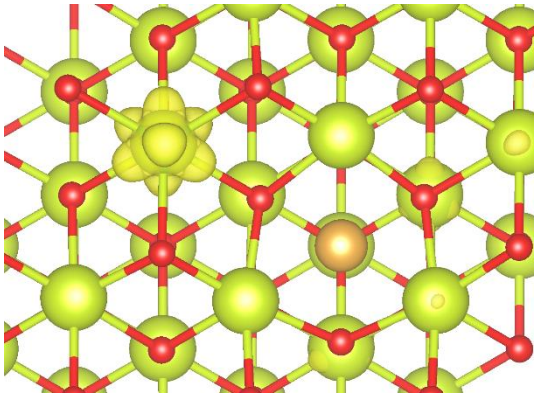


Figure S 11: Iso-surface of the electron density of the highest occupied band of Au_1/CeO_{2-x}; iso-value 0.003 e $Å^{-3}$.

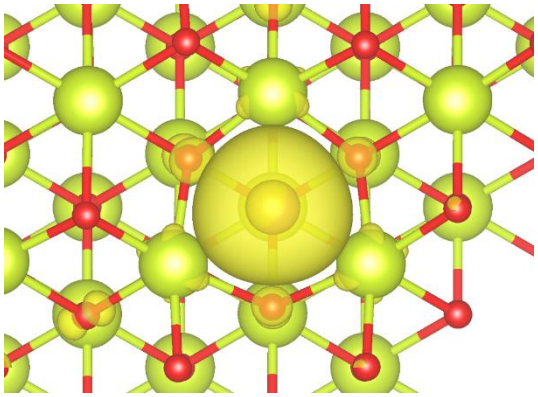


Figure S 12: Iso-surface of the electron density of the second highest occupied band of Au_1/CeO_{2-x}; iso-value 0.003 e $Å^{-3}$.

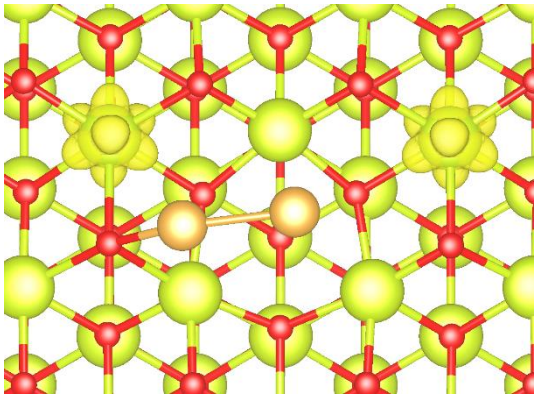


Figure S 13: Iso-surface of spin density (α-β) of Au_2/CeO_{2-x}; iso-value 0.003 e $Å^{-3}$.

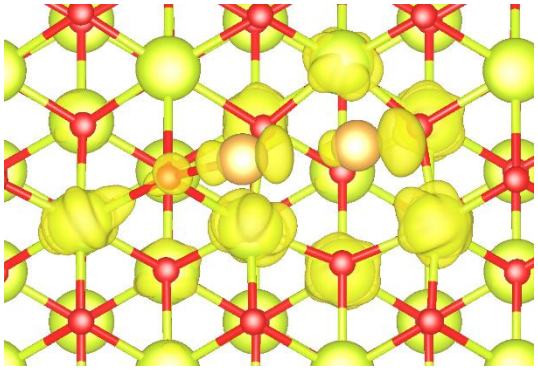


Figure S 14: Iso-surface of the lowest unoccupied band of Au_2/CeO_{2-x}; iso-value 0.003 e $Å^{-3}$.

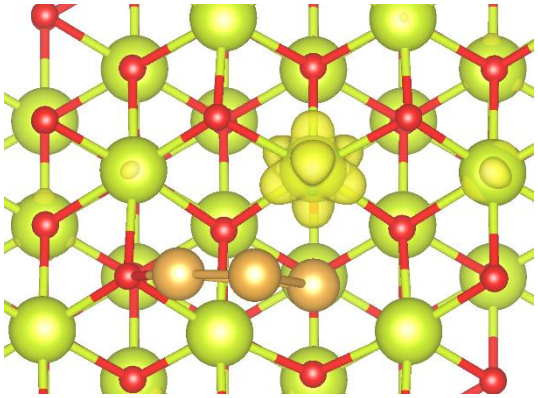


Figure S 15 Iso-surface of the electron density of the highest occupied band of Au_3/CeO_{2-x}; vacancy under Au_3; iso-value 0.003 e $Å^{-3}$.

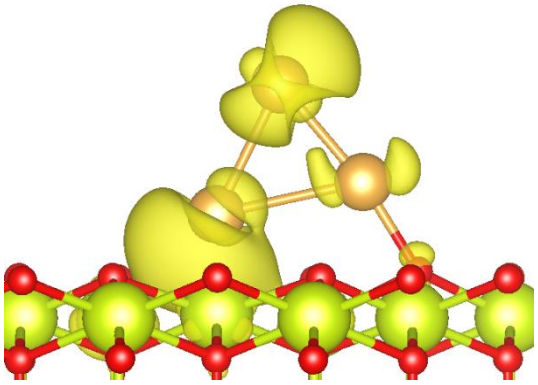


Figure S 16: Iso-surface of the electron density of the second highest occupied band of Au_3/CeO_{2-x}; vacancy under Au_3; isovalue 0.003 e $Å^{-3}$.

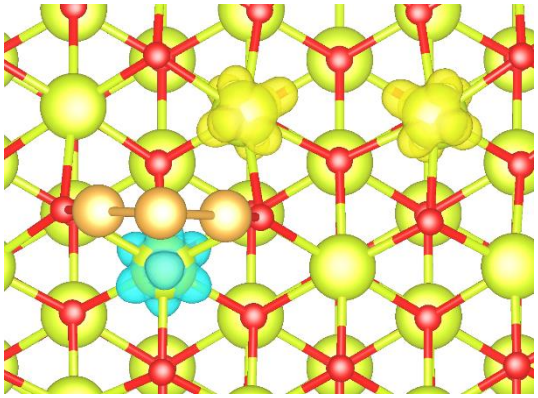


Figure S 17: Iso-surface of spin density (α-β) of Au_3/CeO_{2-x}; vacancy next to cluster; iso-value 0.003 e $Å^{-3}$.

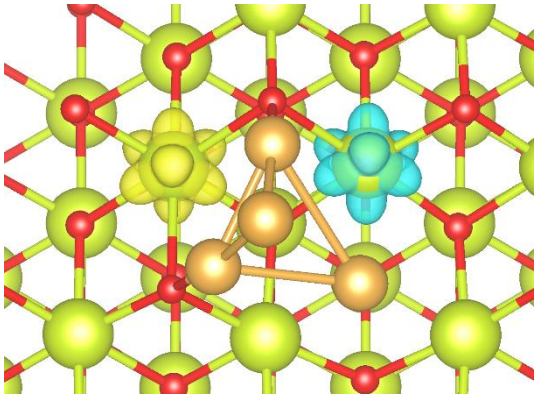


Figure S 18: Spin density (α-β) of Au_4/CeO_{2-x}; iso-value 0.003 e $Å^{-3}$.

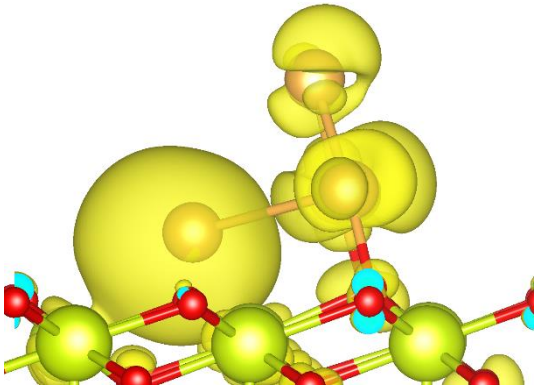


Figure S 19: Iso-surface of the electron density of the third highest occupied band of Au_4/CeO_{2-x}; vacancy under Au_4; isovalue 0.003 e $Å^{-3}$.

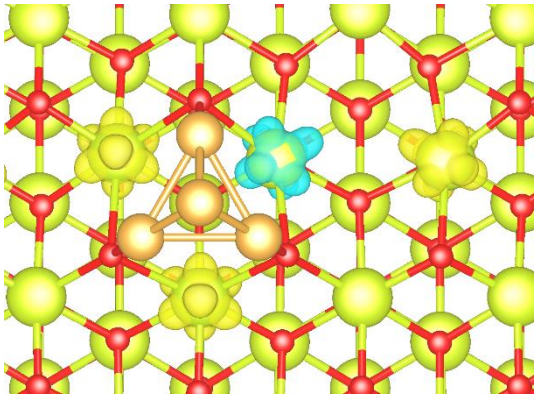


Figure S 20: Spin density (α-β) of Au_4/CeO_{2-x}; vacancy next to Au_4; iso-value 0.003 e $Å^{-3}$.

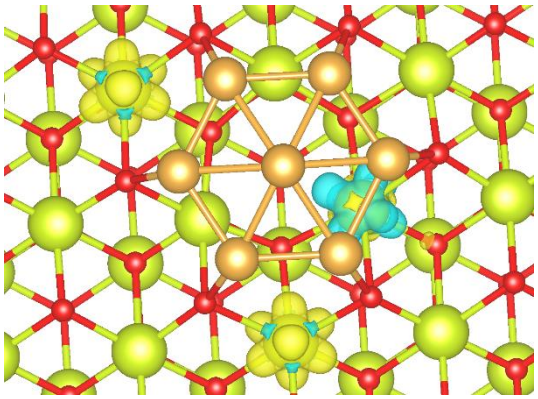


Figure S 21: Spin density (α-β) of Au_7/CeO_{2-x}; vacancy under to Au_7; iso-value 0.003 e $Å^{-3}$.

Au8 a-b density

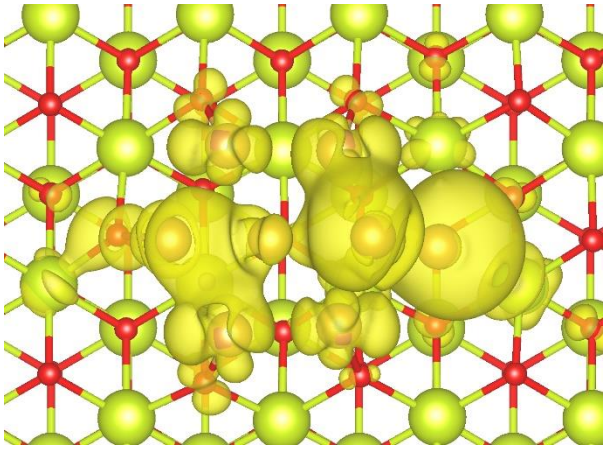


Figure S 22: Iso-surface of the electron density of the fourth highest occupied band of Au_8/CeO_{2-x}; vacancy under corner atom; isovalue 0.003 e $Å^{-3}$.

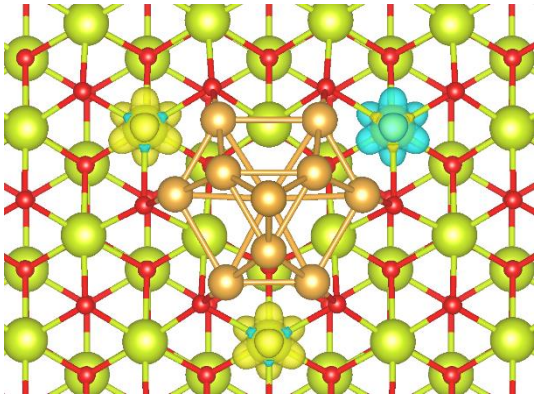


Figure S 23: Spin density (α-β) of Au_{11}/CeO_{2-x}; vacancy under to Au_{11}; iso-value 0.003 e $Å^{-3}$.

2. Electrostatic potential plots

Table S 2: Iso-surfaces of the electron density (iso-value: 0.001 a.u) mapped with the (electrostatic) local potential; colour scale between ≥−2.2 eV (blue) and ≤−4.0 eV (red); isolated Au_8 clusters; structures taken from Au_8/CeO_{2-x}.

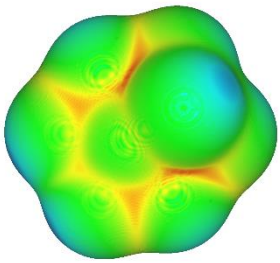
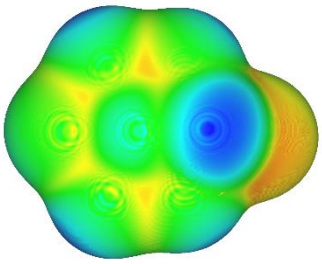
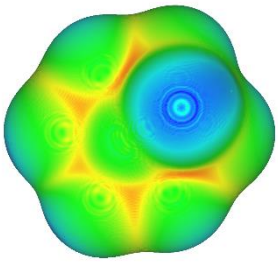
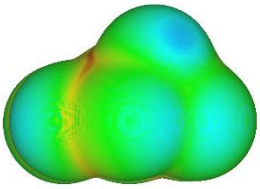
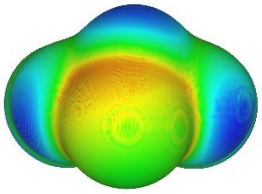
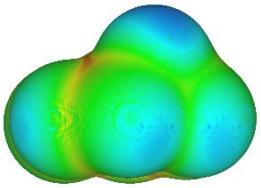
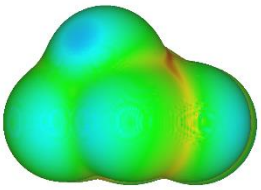
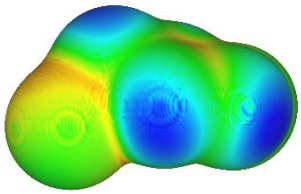
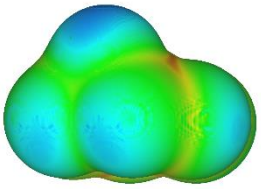
Next	Corner	Under
		
		
		

Table S 3: Iso-surfaces of the electron density (iso-value: 0.001 a.u) mapped with the (electrostatic) local potential; colour scale between ≥−2.0 eV (blue) and ≤−4.5 eV (red); isolated Au_{11} clusters; structures taken from Au_8/CeO_2 and Au_8/CeO_{2-x}.

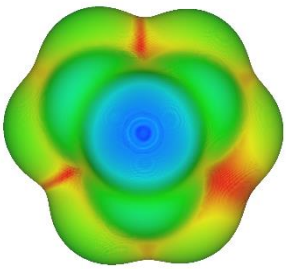
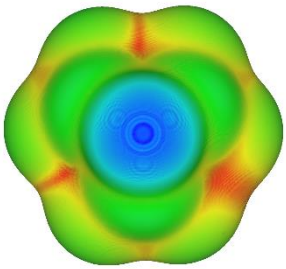
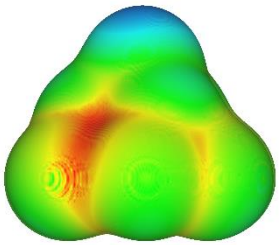
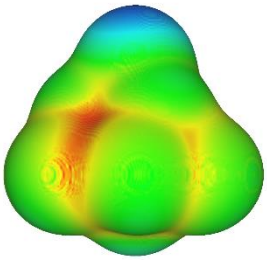
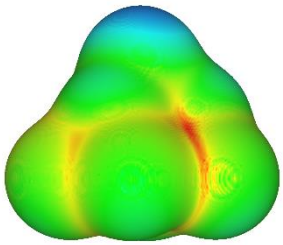
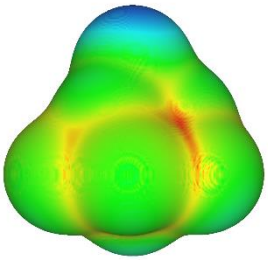
CeO_2	CeO_{2-x}
	
	
	

Table S 4: Iso-surfaces of the electron density (iso-value: 0.001 a.u) mapped with the (electrostatic) local potential; colour scale between ≥−2.0 eV (blue) and ≤−3.8 eV (red); isolated Au_{11} clusters; structures taken from Au_8/CeO_2 and Au_8/CeO_{2-x}.

CeO_2	CeO_{2-x}