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Supporting information

Copper-doped $LaCoO_3$ for Direct Propylene Epoxidation: A DFT Study

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Part S1: Microkinetic modeling

The in-house-developed C++ program MKMCXX was employed to determine the steady-state coverages by integrating this set of ordinary differential equations with respect to time using the backward differentiation formula method. The steady-state surface coverage values were used to compute the rates of the individual elementary reaction steps. For surface reactions, the rate constant k and pre-exponential factors A0 were calculated using the following equation:

$$k = \frac{k_B T}{h} \frac{q_{iv}^{TS}}{q_{iv}^{IS}} exp\left\{\frac{E_{ZP}}{k_B T}\right\} = Aexp\left\{\frac{-E_{ZP}}{k_B T}\right\}.$$

Where k_B, E_{ZP}, q_{iv}^{TS}, q_{iv}^{IS} represent Ludwig Boltzmann's constant, activation energy corrected by zero-point energy, and vibrational partition function of TS (IS) , respectively. The rate constants for adsorption and desorption of species I can be calculated as follows：

$$r'_{ads} = k_{ads} Y_i \theta_*$$

$$r'_{des} = k_{des} \theta_{i*}$$

k_{ads} (k_{des}) , Y_i, θ^* and θ_i^* refer to the rate constants of the adsorption (desorption) process, the mole fraction and mole fraction of the gas phase, and the coverage of vacancies and I, respectively. The following equations are used to calculate k_{ads} and k_{des}:

$$k'_{ads} = \frac{A_{site} P_i \sigma_i}{\sqrt{2\pi m_i k_B T}}$$

$$k'_{des} = \frac{k_B}{h^3} \frac{A(2\pi m_i k_B)}{\sigma \theta_{rot}} exp^{-E_{des}/k_B T}$$

A_{site} is the area of adsorption site, P_i, σ_i and m_i are the partial pressure, viscosity coefficient and mass of component i respectively. σ and θ rot are dimensionless symmetric numbers and characteristic temperatures of rotation, respectively. E_{des} is desorption energy. The rotational characteristic temperature and temperature are calculated by the following formula:

$$\theta_{rot} = \frac{h^3}{8\pi^2 k_B I}$$

Part S2: PDE over CoO, CuCoO, LaO and LaCuO surfaces

Table S1. Adsorption energy (E_{ads}) and adsorption free energy (G_{ads}) of key species involved in Propylene epoxidation on CoO, CuCoO, LaO and LaCuO surfaces.

species	CoO		CoCuO		LaO		LaCuO	
	E_{ads}/eV	G_{ads}/eV	E_{ads}/eV	G_{ads}/eV	E_{ads}/eV	G_{ads}/eV	E_{ads}/eV	G_{ads}/eV
O_2	-0.22	0.28	-0.15	0.35	-0.49	0.02	-0.43	0.07
C_3H_6	-0.80	-0.16	-0.69	-0.05	-0.34	0.30	-0.32	0.32
C_3H_5	-0.99	-0.35	-0.91	-0.27	-0.45	0.19	-0.42	0.22
C_3H_5O	-2.34	-0.99	-2.08	-0.79	-2.85	-1.81	-2.63	-1.06
$OOMMP_1$	-1.17	0.98	-0.96	1.20	-1.22	0.71	-0.80	1.14
$OOMMP_2$	-1.03	1.11	-0.78	1.40	-0.57	1.25	-0.53	1.33
C_3H_4O	-1.21	-0.55	-0.68	-0.02	-0.96	-0.30	-0.42	0.25
PO	-0.78	-0.11	-0.59	0.09	-0.75	-0.07	-0.51	0.16
PA	-0.71	-0.04	-0.89	-0.22	-0.83	-0.16	-0.44	0.24
AC	-1.03	-0.35	-0.61	0.07	-0.77	-0.10	-0.44	0.24

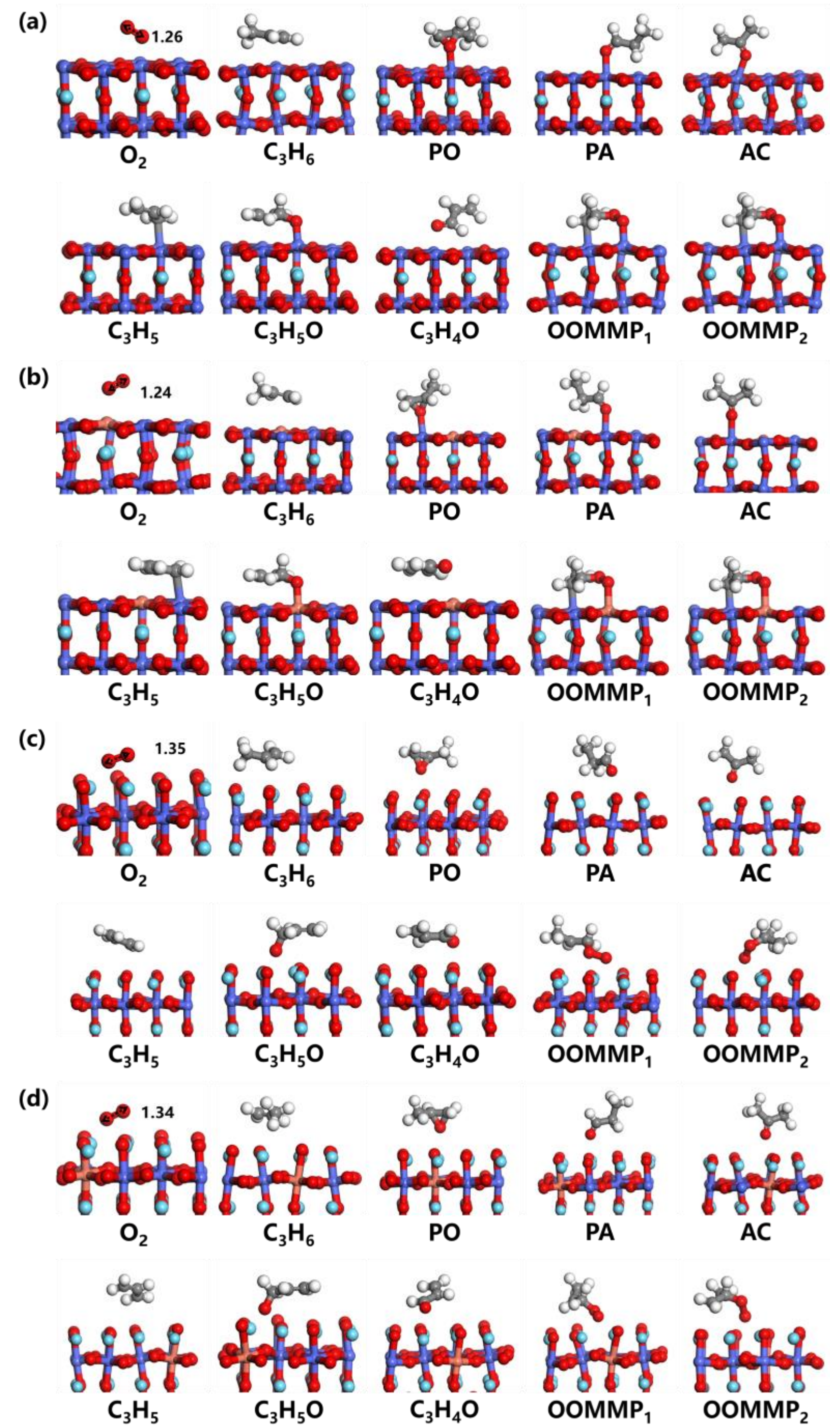

Figure S1. Possible adsorption configuration of key species of propylene epoxidation on CoO (a), CuCoO (b), LaO (c) and LaCuO Surface (d) (unit: Å).

Table S2. Elementary steps and kinetic parameters for the selective oxidation of propylene on CoO surface with molecular O_2.

Elementary reactions	E_a/eV	A	E_a^{-r}/eV	A^{-r}
$C_3H_6^*+O_2^*\rightarrow C_3H_5^*+OOH^*$	1.63	4.28×10^{11}	0.85	4.56×10^{12}
$C_3H_5^*+OOH^*\rightarrow C_3H_5O^*+OH$	1.74	4.69×10^{13}	4.23	6.82×10^{13}
$C_3H_5O^*+OH^*\rightarrow C_3H_4O^*+H_2O^*$	1.00	1.08×10^{13}	2.79	4.56×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_1^*$	1.75	1.24×10^{12}	0.71	4.13×10^{13}
$OOMMP_1^*+^*\rightarrow PO_1^*+O^*$	0.75	7.23×10^{13}	2.93	8.97×10^{12}
$OOMMP_1^*+^*\rightarrow PA^*+O^*$	1.35	2.67×10^{13}	3.01	1.21×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_2^*$	1.65	9.07×10^{11}	0.71	3.30×10^{13}
$OOMMP_2^*+^*\rightarrow PO_2^*+O^*$	1.50	1.97×10^{12}	2.79	7.63×10^{12}
$OOMMP_2^*+^*\rightarrow AC^*+O^*$	1.39	2.90×10^{12}	3.64	3.53×10^{12}
$2O^*\rightarrow O_2^*+*$	1.75	8.64×10^{12}	4.34	1.91×10^{12}

Table S3. Elementary steps and kinetic parameters for the selective oxidation of propylene on CoCuO surface with molecular O_2.

Elementary reactions	E_a/eV	A	E_a^{-r}/eV	A^{-r}
$C_3H_6^*+O_2^*\rightarrow C_3H_5^*+OOH^*$	2.75	4.17×10^{12}	1.15	6.23×10^{12}
$C_3H_5^*+OOH^*\rightarrow C_3H_5O^*+OH$	1.50	4.57×10^{12}	3.53	2.71×10^{13}
$C_3H_5O^*+OH^*\rightarrow C_3H_4O^*+H_2O^*$	1.22	5.14×10^{12}	4.00	2.51×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_1^*$	1.74	3.32×10^{12}	0.39	1.02×10^{14}
$OOMMP_1^*+^*\rightarrow PO_1^*+O^*$	1.71	2.27×10^{13}	1.95	1.74×10^{13}
$OOMMP_1^*+^*\rightarrow PA^*+O^*$	0.96	1.02×10^{13}	1.66	5.04×10^{13}
$C_3H_6^*+O_2^*\rightarrow OOMMP_2^*$	1.59	1.29×10^{12}	0.53	2.79×10^{13}
$OOMMP_2^*+^*\rightarrow PO_2^*+O^*$	1.85	1.84×10^{13}	1.84	6.54×10^{13}
$OOMMP_2^*+^*\rightarrow AC^*+O^*$	1.63	1.19×10^{13}	3.23	4.27×10^{13}
$2O^*\rightarrow O_2^*+*$	1.63	9.18×10^{12}	5.48	3.97×10^{12}

Table S4. Elementary steps and kinetic parameters for the selective oxidation of propylene on LaO surface with molecular O_2.

Elementary reactions	E_a/eV	A	E_a^{-r}/eV	A^{-r}
$C_3H_6^*+O_2^*\rightarrow C_3H_5^*+OOH^*$	0.75	6.31×10^{12}	0.12	9.31×10^{12}
$C_3H_5^*+OOH^*\rightarrow C_3H_5O^*+OH$	1.21	2.28×10^{13}	3.58	9.57×10^{13}
$C_3H_5O^*+OH^*\rightarrow C_3H_4O^*+H_2O^*$	0.67	1.38×10^{13}	1.57	8.01×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_1^*$	0.91	4.20×10^{12}	0.12	2.05×10^{13}
$OOMMP_1^*+^*\rightarrow PO_1^*+O^*$	0.48	1.42×10^{13}	1.59	1.07×10^{13}
$OOMMP_1^*+^*\rightarrow PA^*+O^*$	0.02	3.93×10^{13}	2.35	2.27×10^{13}
$C_3H_6^*+O_2^*\rightarrow OOMMP_2^*$	1.27	3.50×10^{12}	0.08	2.12×10^{13}
$OOMMP_2^*+^*\rightarrow PO_2^*+O^*$	0.06	1.36×10^{13}	1.35	5.62×10^{12}
$OOMMP_2^*+^*\rightarrow AC^*+O^*$	0.52	1.61×10^{13}	3.00	5.69×10^{12}
$2O^*\rightarrow O_2^*+*$	0.36	8.78×10^{12}	1.64	4.03×10^{13}

Table S5. Elementary steps and kinetic parameters for the selective oxidation of propylene on LaCuO surface with molecular O_2.

Elementary reactions	E_a/eV	A	E_a^{-r}/eV	A^{-r}
$C_3H_6^*+O_2^*\rightarrow C_3H_5^*+OOH^*$	0.88	4.67×10^{12}	0.51	2.95×10^{12}
$C_3H_5^*+OOH^*\rightarrow C_3H_5O^*+OH$	0.77	1.17×10^{13}	2.53	5.46×10^{13}
$C_3H_5O^*+OH^*\rightarrow C_3H_4O^*+H_2O^*$	0.17	2.53×10^{13}	1.79	6.85×10^{13}
$C_3H_6^*+O_2^*\rightarrow OOMMP_1^*+^*$	0.78	6.03×10^{12}	0.10	2.00×10^{13}
$OOMMP_1^*+^*\rightarrow PO_1^*+O^*$	0.18	1.94×10^{13}	1.63	1.19×10^{13}
$OOMMP_1^*+^*\rightarrow PA^*+O^*$	0.01	2.75×10^{13}	2.27	1.18×10^{13}
$C_3H_6^*+O_2^*\rightarrow OOMMP_2^*$	0.96	4.21×10^{12}	0.44	1.78×10^{13}
$OOMMP_2^*+^*\rightarrow PO_2^*+O^*$	0.84	1.62×10^{12}	2.22	3.59×10^{12}
$OOMMP_2^*+^*\rightarrow AC^*+O^*$	1.25	6.64×10^{12}	3.52	7.15×10^{12}
$2O^*\rightarrow O_2^*+*$	0.38	1.29×10^{13}	1.61	7.59×10^{12}

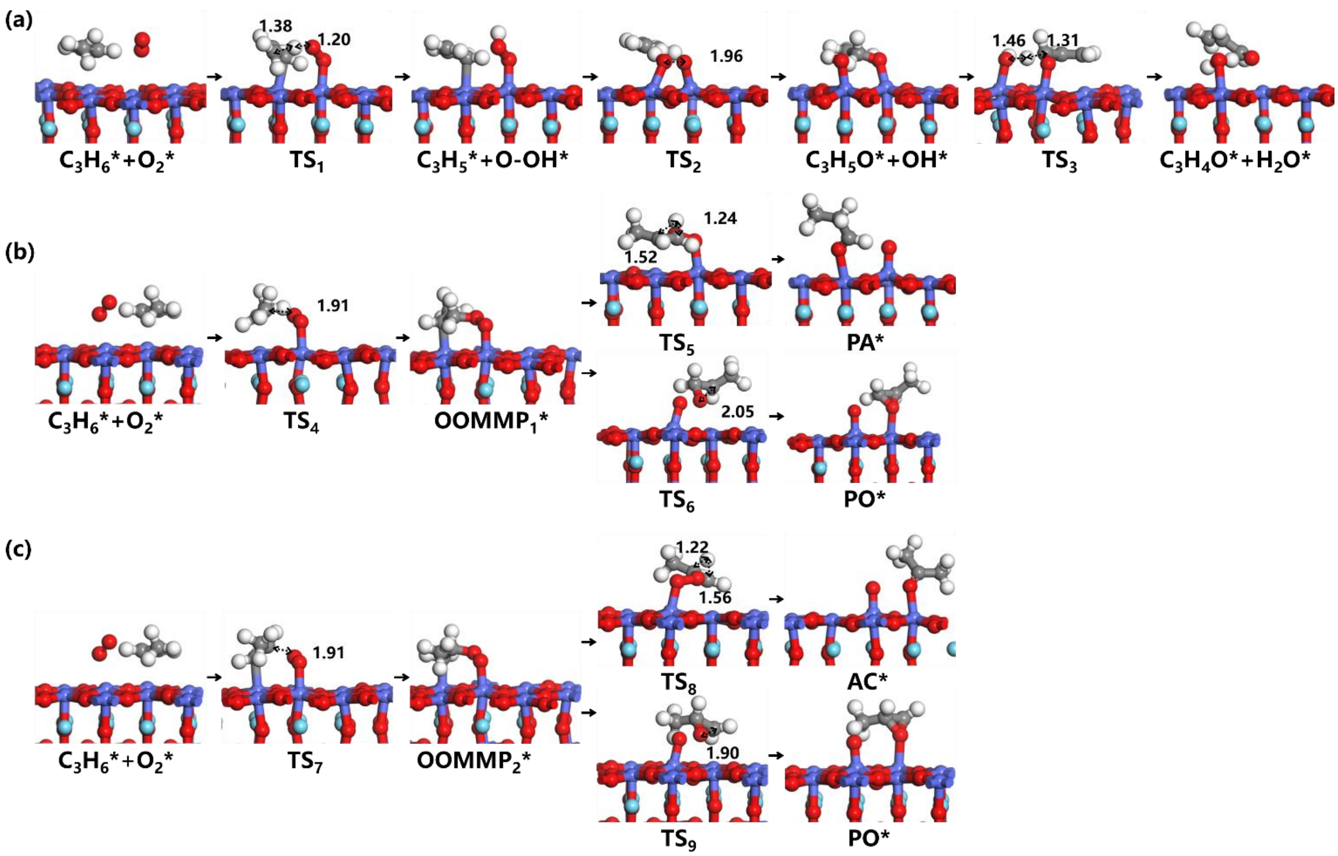

Figure S2. Reaction networks of dehydrogenation (a) and epoxidation (b-c) of propylene with O_2^* as an oxidant on CoO. Bond lengths are in Å.

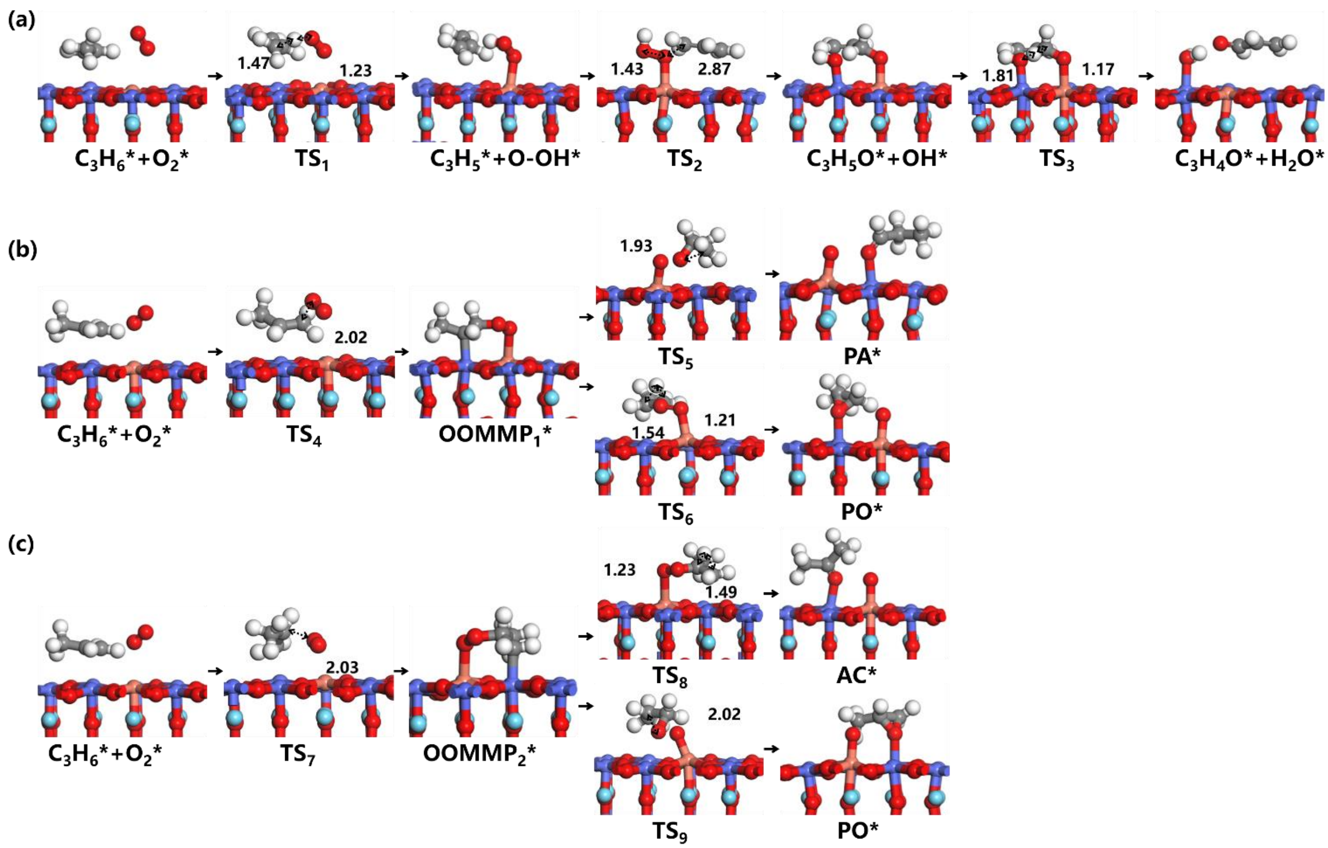

Figure S3. Reaction networks of dehydrogenation (a) and epoxidation (b-c) of propylene with O_2^* as an oxidant on CoCuO. Bond lengths are in Å.

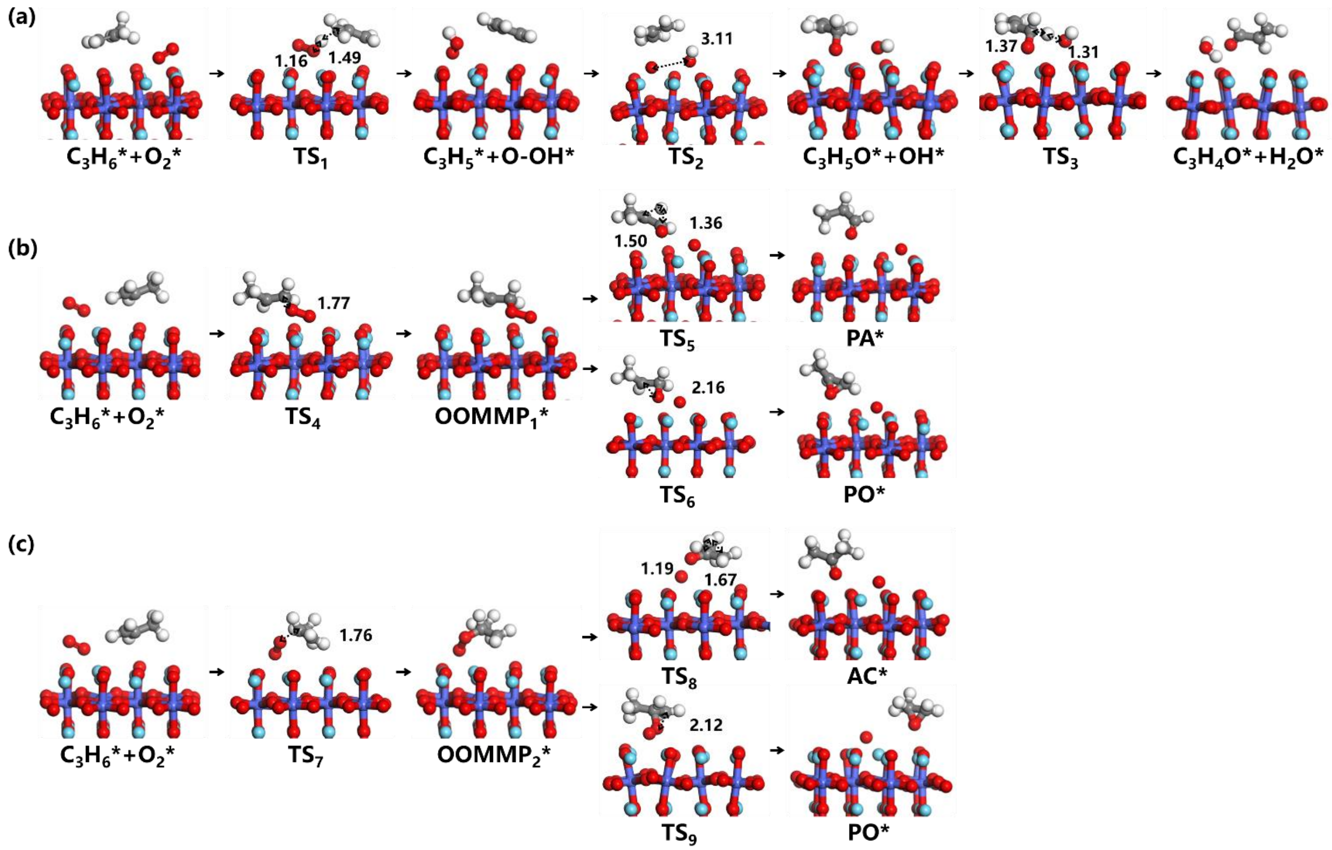

Figure S4. Reaction networks of dehydrogenation (a) and epoxidation (b-c) of propylene with O_2^* as an oxidant on LaO. Bond lengths are in Å.

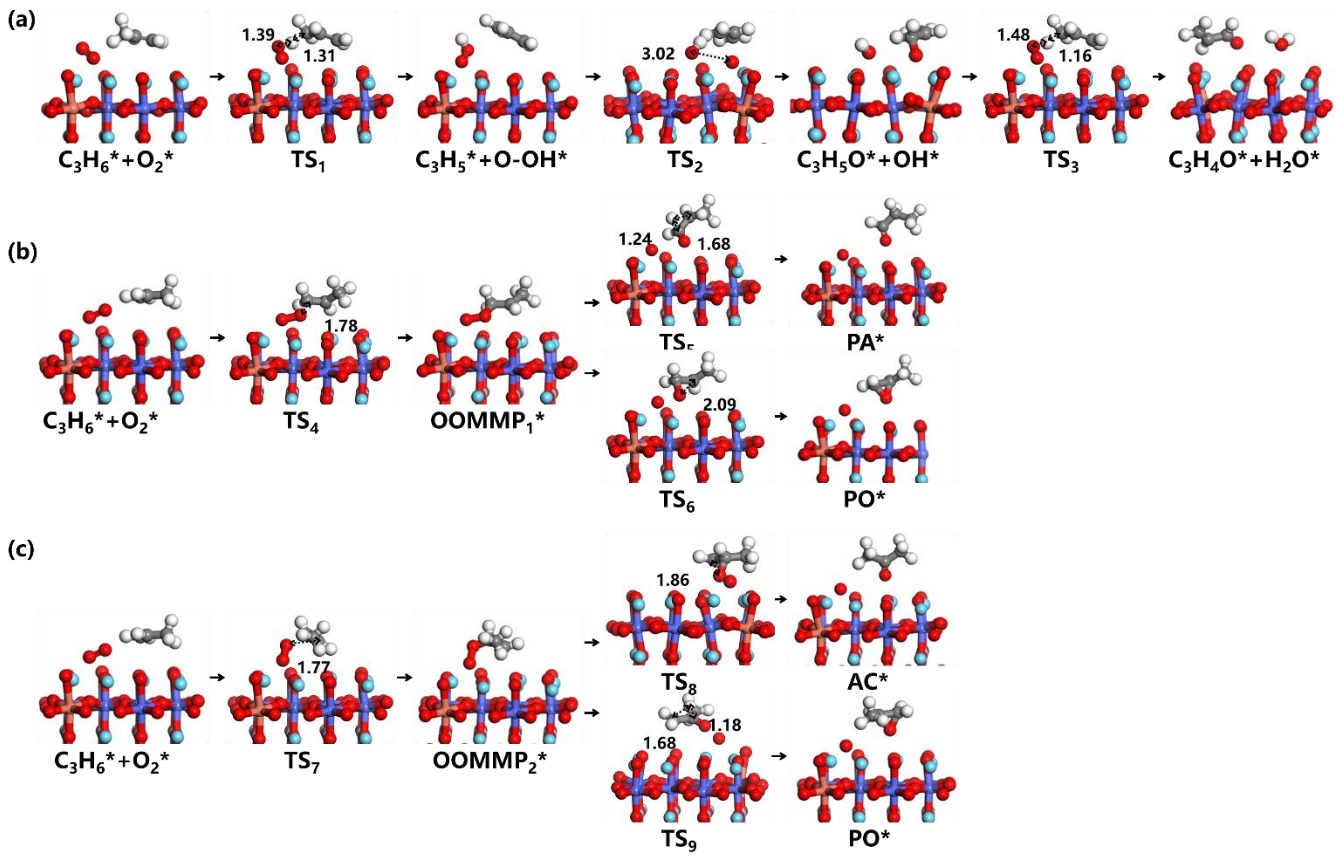

Figure S5. Reaction networks of dehydrogenation (a) and epoxidation (b-c) of propylene with O_2^* as an oxidant on LaCuO. Bond lengths are in Å.

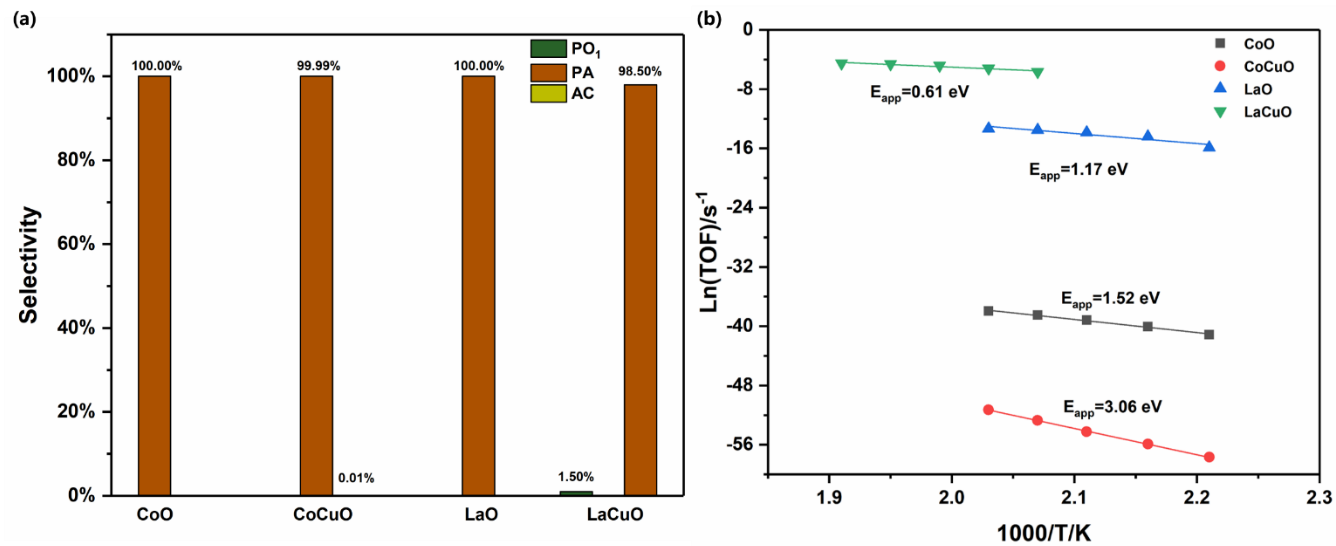

Figure S6. The selectivity of products at 523 K (a) and the apparent activation energies of PO (b) on CoO, CuCoO, LaO and LaCuO surfaces.

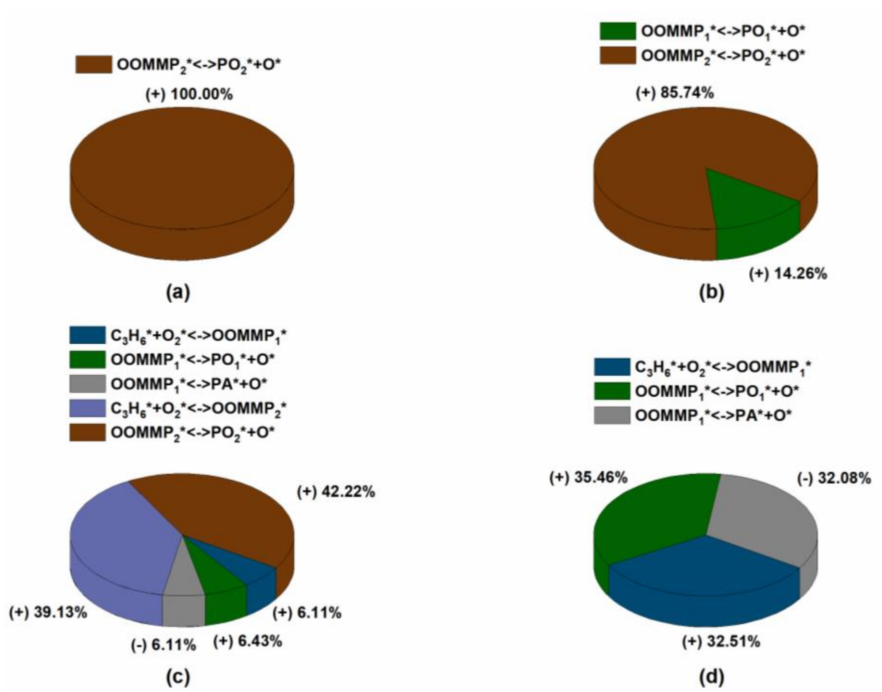

Figure S7. Distribution of the elementary steps toward total PO formation on CoO (a), CoCuO (b), LaO (c) and LaCuO (d). Note: Positive and negative values refer to the promotion and inhibition of the rate, respectively.

Part S3: PDE over CoO-Cl, CoCuO-Cl, LaO-Cl, and LaCuO-Cl surfaces

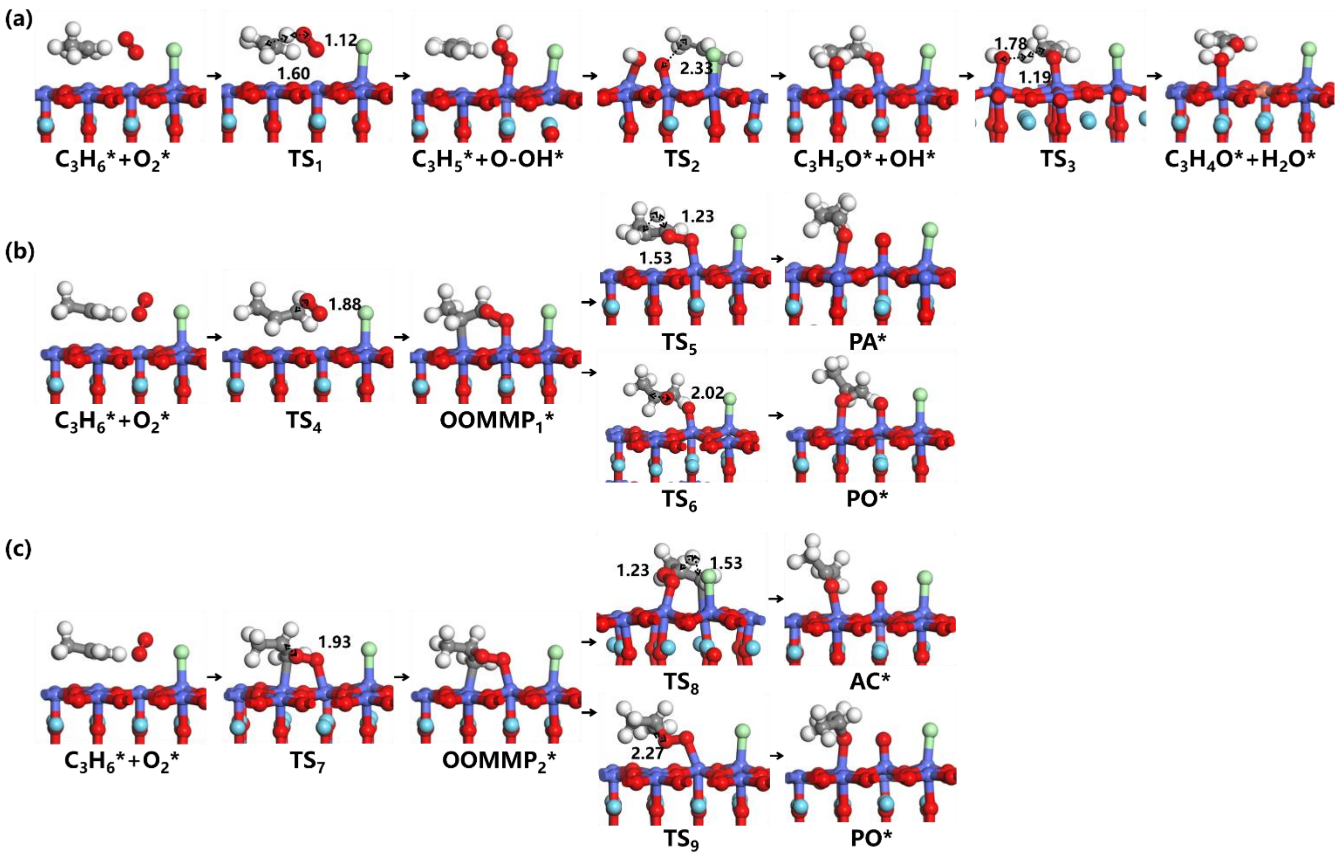

Figure S8. Reaction networks of dehydrogenation (a) and epoxidation (b-c) of propylene with O_2^* as an oxidant on CoO-Cl. Bond lengths are in Å.

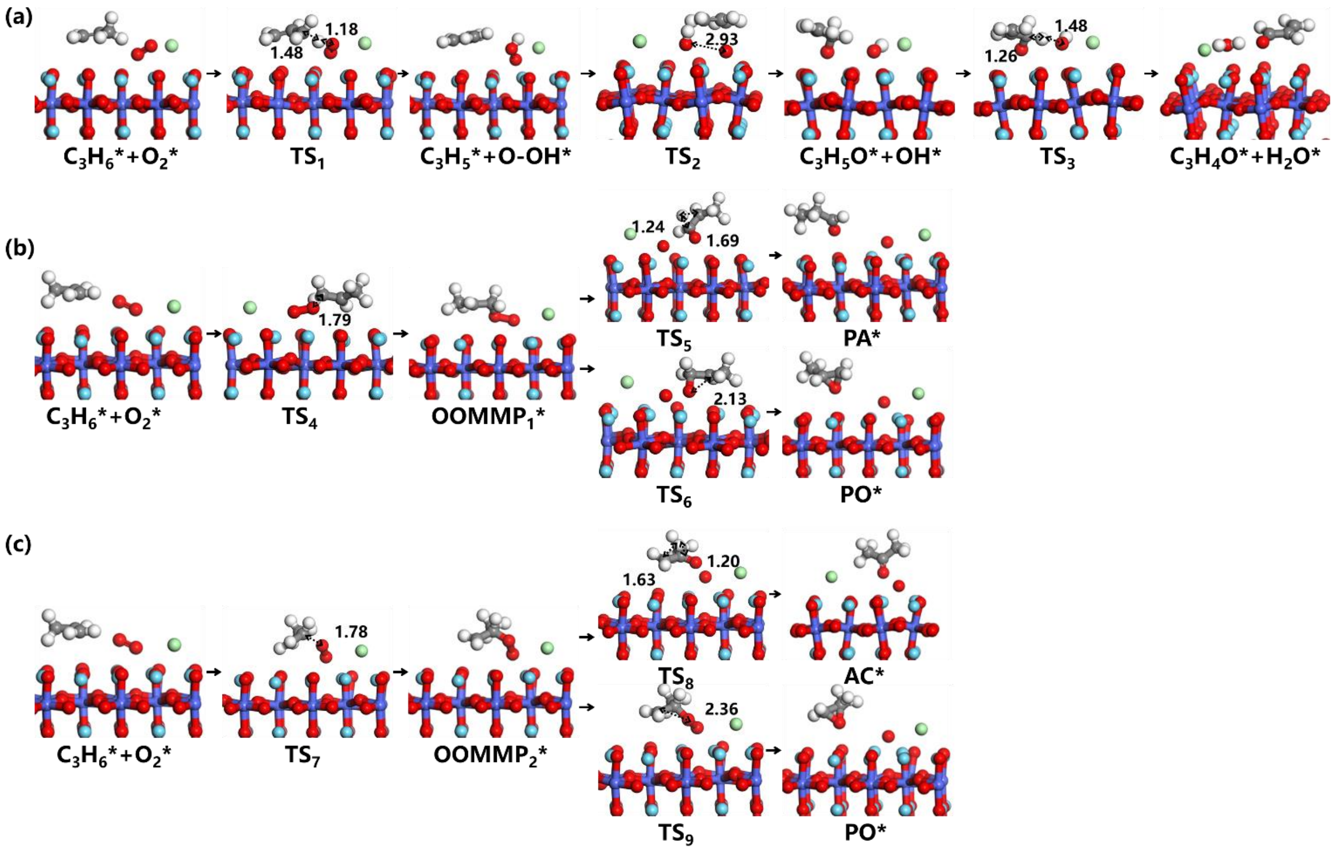

Figure S9. Reaction networks of dehydrogenation (a) and epoxidation (b-c) of propylene with O_2^* as an oxidant on LaO-Cl. Bond lengths are in Å.

Table S6.

The Gibbs free energy barriers (ΔG_a) and reaction free energy (ΔG) of each elemental step of propylene epoxidation on LaCuO-Cl terminated surfaces.

Elementary reactions	ΔG/eV	G_a/eV
$C_3H_6^*$+O^*→$OMMP_1^*$	-0.69	0.75
$OMMP_1^*$+*→PA^*	-1.40	0.50
$OMMP_1^*$+*→PO_1^*	-0.87	0.41
$C_3H_6^*$+O^*→$OMMP_2^*$	-0.53	0.90
$OMMP_2^*$+*→AC^*+O^*	-2.05	0.23
$OMMP_2^*$+*→PO_2^*+O^*	-1.07	0.28

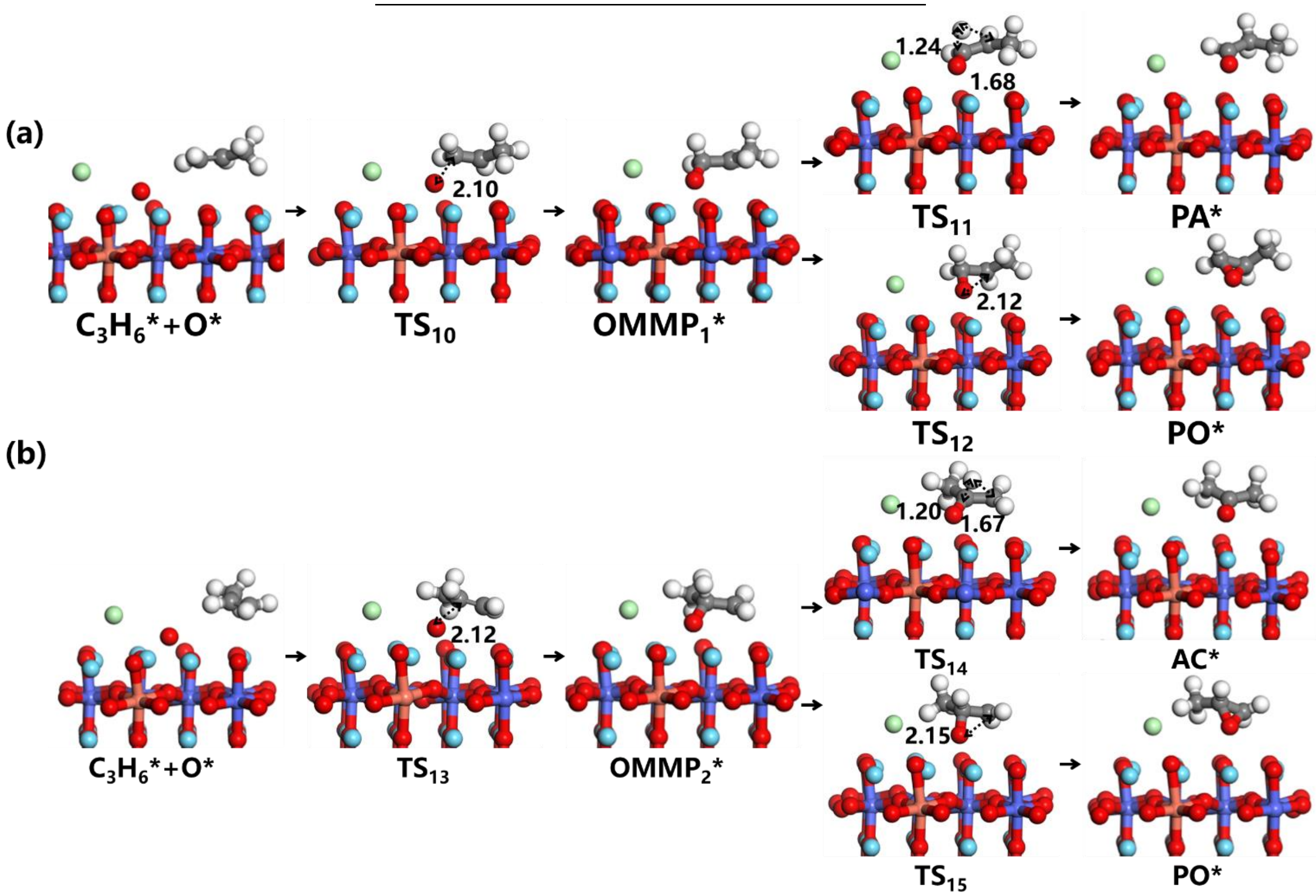

Figure S10. Reaction networks of epoxidation (a-b) of propylene with O^* as an oxidant on LaCuO-Cl. Bond lengths are in Å.

Table S7.

Adsorption energy (E_{ads}) and adsorption free energy (G_{ads}) of key species involved in Propylene epoxidation on CoO-Cl, CoCuO-C, LaO-Cl and LaCuO-Cl surfaces.

species	CoO-Cl		CoCuO-Cl		LaO-Cl		LaCuO-Cl	
	E_{ads}/eV	G_{ads}/eV	E_{ads}/eV	G_{ads}/eV	E_{ads}/eV	G_{ads}/eV	E_{ads}/eV	G_{ads}/eV
O_2	-0.32	0.18	-0.25	0.25	-0.45	0.05	-0.46	0.04
C_3H_6	-1.06	-0.42	-0.99	-0.35	-0.50	0.14	-0.65	-0.10
C_3H_5	-1.22	-0.58	-0.90	-0.26	-0.47	0.17	-0.43	0.21
C_3H_5O	-2.13	-0.86	-1.96	-0.60	-2.25	-1.23	-2.41	-1.06
$OOMMP_1$	-0.58	1.48	-0.67	1.44	-0.77	1.00	-0.82	1.03
$OOMMP_2$	-0.81	1.22	-0.52	1.60	-0.62	1.38	-0.52	1.13
C_3H_4O	-1.33	-0.67	-1.21	-0.55	-0.93	-0.26	-0.66	0.01
PO	-0.60	0.07	-0.91	-0.24	-0.84	-0.16	-0.67	0.01
PA	-0.67	0.01	-1.06	-0.39	-1.05	-0.38	-0.79	-0.12
AC	-0.94	-0.26	-1.12	-0.44	-1.17	-0.49	-0.51	0.17

Table S8.

Elementary steps and kinetic parameters for the selective oxidation of propylene on CoO-Cl surface with molecular O_2.

Elementary reactions	E_a/eV	A	E_a^{-r}/eV	A^{-r}
$C_3H_6^*+O_2^*\rightarrow C_3H_5^*+OOH^*$	1.58	1.12×10^{13}	0.85	2.81×10^{13}
$C_3H_5^*+OOH^*\rightarrow C_3H_5O^*+OH$	0.56	5.91×10^{12}	3.07	1.73×10^{13}
$C_3H_5O^*+OH^*\rightarrow C_3H_4O^*+H_2O^*$	1.26	6.55×10^{12}	2.84	3.97×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_1^*$	0.89	2.46×10^{12}	0.49	4.77×10^{13}
$OOMMP_1^*+^*\rightarrow PO_1^*+O^*$	1.16	3.79×10^{13}	1.94	4.84×10^{13}
$OOMMP_1^*+^*\rightarrow PA^*+O^*$	0.54	2.75×10^{13}	1.74	9.81×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_2^*$	0.71	1.90×10^{12}	0.68	2.28×10^{13}
$OOMMP_2^*+^*\rightarrow PO_2^*+O^*$	0.99	7.67×10^{12}	1.29	8.13×10^{12}
$OOMMP_2^*+^*\rightarrow AC^*+O^*$	1.24	7.13×10^{12}	2.66	6.36×10^{12}
$2O^*\rightarrow O_2^*+*$	1.24	1.61×10^{13}	3.79	9.27×10^{12}

Table S9.

Elementary steps and kinetic parameters for the selective oxidation of propylene on CoCuO-Cl surface with molecular O_2.

Elementary reactions	E_a/eV	A	E_a^{-r}/eV	A^{-r}
$C_3H_6^*+O_2^*\rightarrow C_3H_5^*+OOH^*$	2.04	2.92×10^{12}	1.34	4.81×10^{12}
$C_3H_5^*+OOH^*\rightarrow C_3H_5O^*+OH$	1.27	3.53×10^{12}	3.19	4.32×10^{13}
$C_3H_5O^*+OH^*\rightarrow C_3H_4O^*+H_2O^*$	0.77	1.60×10^{13}	3.69	4.48×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_1^*$	1.33	2.68×10^{12}	0.22	3.25×10^{13}
$OOMMP_1^*+^*\rightarrow PO_1^*+O^*$	0.69	4.05×10^{13}	1.70	2.41×10^{12}
$OOMMP_1^*+^*\rightarrow PA^*+O^*$	0.67	3.25×10^{13}	2.58	7.39×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_2^*$	1.60	2.50×10^{12}	0.40	4.48×10^{13}
$OOMMP_2^*+^*\rightarrow PO_2^*+O^*$	1.70	6.76×10^{12}	2.78	3.12×10^{13}
$OOMMP_2^*+^*\rightarrow AC^*+O^*$	0.54	1.53×10^{13}	2.55	2.89×10^{12}
$2O^*\rightarrow O_2^*+*$	0.36	5.30×10^{12}	1.64	2.56×10^{12}

Table S10.

Elementary steps and kinetic parameters for the selective oxidation of propylene on LaO-Cl surface with molecular O_2.

Elementary reactions	E_a/eV	A	E_a^{-r}/eV	A^{-r}
$C_3H_6^*+O_2^*\rightarrow C_3H_5^*+OOH^*$	0.82	5.07×10^{12}	0.12	1.20×10^{13}
$C_3H_5^*+OOH^*\rightarrow C_3H_5O^*+OH$	0.34	4.45×10^{13}	3.47	1.18×10^{14}
$C_3H_5O^*+OH^*\rightarrow C_3H_4O^*+H_2O^*$	0.63	1.44×10^{13}	2.14	9.12×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_1^*+^*$	0.74	6.21×10^{12}	0.46	2.36×10^{13}
$OOMMP_1^*+^*\rightarrow PO_1^*+O^*$	0.64	1.05×10^{13}	2.06	7.30×10^{12}
$OOMMP_1^*+^*\rightarrow PA^*+O^*$	0.60	2.02×10^{13}	2.26	3.40×10^{13}
$C_3H_6^*+O_2^*\rightarrow OOMMP_2^*$	0.77	5.87×10^{12}	0.09	4.38×10^{13}
$OOMMP_2^*+^*\rightarrow PO_2^*+O^*$	0.25	2.55×10^{13}	2.02	2.40×10^{12}
$OOMMP_2^*+^*\rightarrow AC^*+O^*$	0.74	1.36×10^{13}	3.03	6.39×10^{12}
$2O^*\rightarrow O_2^*+*$	0.02	1.10×10^{13}	1.35	7.50×10^{12}

Table S11.

Elementary steps and kinetic parameters for the selective oxidation of propylene on LaCuO-Cl surface with molecular O_2.

Elementary reactions	E_a/eV	A	E_a^{-r}/eV	A^{-r}
$C_3H_6^*+O_2^*\rightarrow C_3H_5^*+OOH^*$	1.09	4.46×10^{12}	0.38	3.21×10^{12}
$C_3H_5^*+OOH^*\rightarrow C_3H_5O^*+OH$	0.87	1.14×10^{13}	3.32	5.78×10^{13}
$C_3H_5O^*+OH^*\rightarrow C_3H_4O^*+H_2O^*$	1.27	2.94×10^{13}	3.35	7.67×10^{12}
$C_3H_6^*+O_2^*\rightarrow OOMMP_1^*$	0.97	9.92×10^{12}	0.44	1.75×10^{13}
$OOMMP_1^*+^*\rightarrow PO_1^*+O^*$	0.26	8.40×10^{12}	1.55	1.05×10^{13}
$OOMMP_1^*+^*\rightarrow PA^*+O^*$	0.37	1.65×10^{13}	2.38	1.59×10^{13}
$C_3H_6^*+O_2^*\rightarrow OOMMP_2^*$	0.77	4.51×10^{12}	0.12	1.34×10^{13}
$OOMMP_2^*+^*\rightarrow PO_2^*+O^*$	0.47	1.22×10^{13}	2.06	4.47×10^{12}
$OOMMP_2^*+^*\rightarrow AC^*+O^*$	0.96	1.27×10^{13}	3.52	3.30×10^{12}
$C_3H_6^*+O^*\rightarrow OMMP_1^*$	0.75	6.65×10^{12}	1.36	8.93×10^{12}
$OMMP_1^*+^*\rightarrow PO_1^*$	0.41	1.05×10^{13}	1.75	1.50×10^{13}
$OMMP_1^*+^*\rightarrow PA^*$	0.46	4.02×10^{12}	1.84	9.22×10^{12}
$C_3H_6^*+O^*\rightarrow OMMP_2^*$	0.92	1.09×10^{13}	1.34	5.51×10^{13}
$OMMP_2^*+^*\rightarrow PO_2^*$	0.20	4.84×10^{13}	1.34	1.04×10^{13}
$OMMP_2^*+^*\rightarrow AC^*$	0.12	3.92×10^{13}	2.21	7.71×10^{12}
$2O^*\rightarrow O_2^*+*$	0.64	1.10×10^{13}	1.14	4.07×10^{12}

Part S4: The results of frequency analysis of transition states

Table S12.

The results of frequency analysis of transition states on CoO surface

TS_1		TS_2		TS_3		TS_4		TS_7		TS_5		TS_6		TS_8		TS_9	
1f	3172.2	1f	3700.9	1f	3638.8	1f	3142.2	1f	3158.3	1f	3100.7	1f	3099.8	1f	3099.8	1f	3197.6
2f	3122.6	2f	3189.8	2f	3162.3	2f	3085.0	2f	3074.7	2f	3087.3	2f	3059.1	2f	3059.1	2f	3081.2
3f	3070.4	3f	3153.2	3f	3081.2	3f	3045.4	3f	3056.4	3f	3066.5	3f	3005.6	3f	3005.6	3f	3060.4
4f	3051.1	4f	3088.6	4f	3064.8	4f	3026.6	4f	3044.6	4f	3020.4	4f	2981.8	4f	2981.8	4f	3033.3
5f	3015.9	5f	3082.9	5f	2837.0	5f	3012.1	5f	3036.1	5f	2951.0	5f	2931.3	5f	2931.3	5f	2979.8
6f	1505.0	6f	3008.7	6f	1575.9	6f	2938.7	6f	2976.9	6f	2187.6	6f	2893.3	6f	2893.3	6f	2956.1
7f	1454.7	7f	1505.7	7f	1393.5	7f	1451.6	7f	1445.2	7f	1449.8	7f	1458.2	7f	1458.2	7f	1448.6
8f	1398.0	8f	1473.7	8f	1378.1	8f	1435.9	8f	1430.4	8f	1410.6	8f	1436.6	8f	1436.6	8f	1429.0
9f	1370.2	9f	1392.5	9f	1295.8	9f	1405.3	9f	1413.3	9f	1378.2	9f	1408.6	9f	1408.6	9f	1383.0
10f	1257.1	10f	1260.4	10f	1265.0	10f	1365.2	10f	1373.0	10f	1349.5	10f	1369.2	10f	1369.2	10f	1352.0
11f	1221.8	11f	1213.0	11f	1254.7	11f	1336.5	11f	1331.6	11f	1328.7	11f	1331.4	11f	1331.4	11f	1321.9
12f	1185.2	12f	1019.1	12f	1224.7	12f	1201.3	12f	1204.7	12f	1234.8	12f	1253.4	12f	1253.4	12f	1220.6
13f	1033.6	13f	986.0	13f	1033.5	13f	1162.5	13f	1172.5	13f	1155.5	13f	1164.6	13f	1164.6	13f	1149.5
14f	996.0	14f	926.1	14f	998.1	14f	1127.3	14f	1147.5	14f	1146.3	14f	1158.2	14f	1158.2	14f	1120.5
15f	988.1	15f	885.6	15f	920.0	15f	1020.9	15f	1012.4	15f	1033.7	15f	1119.3	15f	1119.3	15f	1053.0
16f	938.9	16f	850.8	16f	912.6	16f	977.3	16f	944.0	16f	1007.5	16f	1032.2	16f	1032.2	16f	911.9
17f	887.6	17f	737.0	17f	858.8	17f	947.4	17f	928.6	17f	945.9	17f	942.0	17f	942.0	17f	885.3
18f	867.7	18f	572.8	18f	801.7	18f	901.1	18f	907.0	18f	885.8	18f	912.3	18f	912.3	18f	844.8
19f	684.8	19f	523.8	19f	677.5	19f	821.7	19f	838.4	19f	833.7	19f	870.6	19f	870.6	19f	792.2
20f	635.9	20f	497.2	20f	576.7	20f	730.8	20f	647.6	20f	708.6	20f	669.5	20f	669.5	20f	641.7
21f	509.8	21f	431.2	21f	553.8	21f	441.9	21f	483.1	21f	600.7	21f	490.7	21f	490.7	21f	523.6
22f	416.8	22f	426.7	22f	457.7	22f	373.7	22f	419.0	22f	442.7	22f	394.0	22f	394.0	22f	461.4
23f	343.3	23f	335.8	23f	363.4	23f	336.5	23f	389.2	23f	402.3	23f	340.2	23f	340.2	23f	393.7
24f	288.1	24f	207.2	24f	345.0	24f	316.5	24f	305.1	24f	350.4	24f	245.3	24f	245.3	24f	369.8
25f	243.6	25f	181.1	25f	311.2	25f	188.6	25f	255.2	25f	200.5	25f	202.1	25f	202.1	25f	247.6
26f	207.0	26f	158.7	26f	242.7	26f	158.8	26f	211.9	26f	184.1	26f	148.4	26f	148.4	26f	230.2
27f	172.7	27f	114.2	27f	150.7	27f	125.4	27f	176.1	27f	168.8	27f	103.2	27f	103.2	27f	203.4
28f	140.9	28f	88.8	28f	129.7	28f	115.8	28f	103.3	28f	126.6	28f	86.0	28f	86.0	28f	167.4
29f	113.7	29f	51.0	29f	121.4	29f	102.3	29f	89.8	29f	106.0	29f	70.3	29f	70.3	29f	98.0
30f	80.9	30f	24.7	30f	106.7	30f	66.4	30f	62.0	30f	94.1	30f	38.7	30f	38.7	30f	89.3
31f	63.0	31f/i	22.6	31f	77.3	31f	53.7	31f	54.3	31f	75.7	31f	25.5	31f	25.5	31f	59.8
32f	53.1	32f/i	40.4	32f	61.9	32f/i	14.7	32f	16.3	32f	24.8	32f/i	36.6	32f/i	36.6	32f	44.4
33f/i	1327.6	33f/i	466.5	33f/i	1251.7	33f/i	462.9	33f/i	352.0	33f/i	1017.1	33f/i	561.4	33f/i	561.4	33f/i	649.3

Table S13.

The results of frequency analysis of transition states on CoCuO surface

TS_1		TS_2		TS_3		TS_4		TS_7		TS_5		TS_6		TS_8		TS_9	
1f	3091.1	1f	3124.1	1f	3193.7	1f	3197.8	1f	3151.7	1f	3091.1	1f	3124.1	1f	3193.7	1f	3197.8
2f	3073.7	2f	3079.1	2f	3074.6	2f	3077.9	2f	3075.3	2f	3073.7	2f	3079.1	2f	3074.6	2f	3077.9
3f	3062.9	3f	3026.7	3f	3072.6	3f	3075.1	3f	3056.6	3f	3062.9	3f	3026.7	3f	3072.6	3f	3075.1
4f	3004.6	4f	3002.2	4f	3044.8	4f	3061.3	4f	3038.0	4f	3004.6	4f	3002.2	4f	3044.8	4f	3061.3
5f	2948.6	5f	2948.2	5f	2973.0	5f	2978.8	5f	3031.5	5f	2948.6	5f	2948.2	5f	2973.0	5f	2978.8
6f	2202.0	6f	2901.8	6f	2163.4	6f	2957.3	6f	2966.7	6f	2202.0	6f	2901.8	6f	2163.4	6f	2957.3
7f	1454.2	7f	1456.8	7f	1433.1	7f	1447.7	7f	1449.8	7f	1454.2	7f	1456.8	7f	1433.1	7f	1447.7
8f	1404.0	8f	1429.9	8f	1398.4	8f	1429.5	8f	1434.6	8f	1404.0	8f	1429.9	8f	1398.4	8f	1429.5
9f	1399.5	9f	1394.8	9f	1380.6	9f	1405.4	9f	1410.7	9f	1399.5	9f	1394.8	9f	1380.6	9f	1405.4
10f	1338.6	10f	1356.8	10f	1363.5	10f	1363.6	10f	1369.3	10f	1338.6	10f	1356.8	10f	1363.5	10f	1363.6
11f	1241.5	11f	1320.1	11f	1289.2	11f	1335.5	11f	1337.5	11f	1241.5	11f	1320.1	11f	1289.2	11f	1335.5
12f	1190.0	12f	1247.9	12f	1253.7	12f	1236.3	12f	1284.1	12f	1190.0	12f	1247.9	12f	1253.7	12f	1236.3
13f	1181.3	13f	1183.6	13f	1120.9	13f	1156.7	13f	1186.5	13f	1181.3	13f	1183.6	13f	1120.9	13f	1156.7
14f	1148.8	14f	1154.3	14f	1042.4	14f	1122.4	14f	1142.5	14f	1148.8	14f	1154.3	14f	1042.4	14f	1122.4
15f	1106.4	15f	1120.5	15f	992.9	15f	1039.3	15f	993.7	15f	1106.4	15f	1120.5	15f	992.9	15f	1039.3
16f	1008.0	16f	1031.5	16f	962.2	16f	912.0	16f	934.1	16f	1008.0	16f	1031.5	16f	962.2	16f	912.0
17f	955.1	17f	938.8	17f	896.6	17f	866.4	17f	908.5	17f	955.1	17f	938.8	17f	896.6	17f	866.4
18f	892.1	18f	903.5	18f	841.5	18f	833.8	18f	889.8	18f	892.1	18f	903.5	18f	841.5	18f	833.8
19f	804.6	19f	875.8	19f	806.2	19f	799.7	19f	768.7	19f	804.6	19f	875.8	19f	806.2	19f	799.7
20f	775.0	20f	688.8	20f	631.9	20f	582.0	20f	602.7	20f	775.0	20f	688.8	20f	631.9	20f	582.0
21f	467.6	21f	445.9	21f	577.3	21f	444.8	21f	429.8	21f	467.6	21f	445.9	21f	577.3	21f	444.8
22f	444.3	22f	403.7	22f	518.7	22f	420.4	22f	382.2	22f	444.3	22f	403.7	22f	518.7	22f	420.4
23f	309.8	23f	354.0	23f	359.3	23f	352.0	23f	330.7	23f	309.8	23f	354.0	23f	359.3	23f	352.0
24f	270.6	24f	234.9	24f	313.1	24f	330.3	24f	205.5	24f	270.6	24f	234.9	24f	313.1	24f	330.3
25f	217.7	25f	175.1	25f	250.8	25f	190.2	25f	178.8	25f	217.7	25f	175.1	25f	250.8	25f	190.2
26f	200.2	26f	167.7	26f	230.6	26f	167.0	26f	164.0	26f	200.2	26f	167.7	26f	230.6	26f	167.0
27f	155.3	27f	127.6	27f	172.0	27f	153.5	27f	123.4	27f	155.3	27f	127.6	27f	172.0	27f	153.5
28f	149.0	28f	83.8	28f	102.1	28f	117.7	28f	106.1	28f	149.0	28f	83.8	28f	102.1	28f	117.7
29f	112.5	29f	54.7	29f	93.8	29f	88.6	29f	70.2	29f	112.5	29f	54.7	29f	93.8	29f	88.6
30f	68.8	30f	46.5	30f	63.5	30f	62.9	30f	54.6	30f	68.8	30f	46.5	30f	63.5	30f	62.9
31f	54.8	31f/i	24.6	31f	58.8	31f	35.8	31f	38.8	31f	54.8	31f/i	24.6	31f	58.8	31f	35.8
32f	20.8	32f/i	120.2	32f/i	37.0	32f	28.9	32f	91.0	32f	20.8	32f/i	120.2	32f/i	37.0	32f	28.9
33f/i	1366.1	33f/i	559.7	33f/i	1202.7	33f/i	668.0	33f/i	709.0	33f/i	1366.1	33f/i	559.7	33f/i	1202.7	33f/i	668.0

Table S14.

The results of frequency analysis of transition states on CoO-Cl surface

TS_1		TS_2		TS_3		TS_4		TS_7		TS_5		TS_6		TS_8		TS_9	
1f	3172.1	1f	3681.5	1f	3682.2	1f	3156.8	1f	3148.7	1f	3106.4	1f	3089.0	1f	3192.3	1f	3198.9
2f	3111.0	2f	3198.8	2f	3157.0	2f	3095.4	2f	3090.4	2f	3093.3	2f	3080.9	2f	3086.9	2f	3096.8
3f	3070.5	3f	3162.3	3f	3083.6	3f	3086.9	3f	3077.0	3f	3080.7	3f	3038.8	3f	3082.2	3f	3067.7
4f	3066.0	4f	3129.6	4f	3072.1	4f	3053.0	4f	3034.7	4f	3067.6	4f	2979.2	4f	3067.2	4f	3053.0
5f	2989.6	5f	3106.5	5f	2847.0	5f	3017.1	5f	3022.6	5f	3013.9	5f	2973.1	5f	3058.3	5f	3038.9
6f	1540.1	6f	3075.9	6f	2014.0	6f	2967.1	6f	3018.4	6f	2189.4	6f	2964.3	6f	2115.0	6f	3009.5
7f	1508.8	7f	1535.1	7f	1588.0	7f	1451.4	7f	1446.8	7f	1444.2	7f	1428.2	7f	1454.6	7f	1444.6
8f	1442.1	8f	1468.8	8f	1411.1	8f	1441.9	8f	1430.6	8f	1436.6	8f	1418.7	8f	1427.1	8f	1427.1
9f	1392.0	9f	1386.1	9f	1306.8	9f	1414.6	9f	1401.0	9f	1396.4	9f	1408.3	9f	1394.9	9f	1412.6
10f	1313.1	10f	1298.5	10f	1280.5	10f	1370.3	10f	1362.8	10f	1363.2	10f	1391.4	10f	1362.8	10f	1348.2
11f	1279.1	11f	1208.3	11f	1266.6	11f	1341.2	11f	1326.1	11f	1247.1	11f	1320.4	11f	1320.2	11f	1302.7
12f	1198.3	12f	1034.6	12f	1159.5	12f	1254.4	12f	1211.0	12f	1210.6	12f	1227.4	12f	1245.1	12f	1190.8
13f	1070.5	13f	993.5	13f	1089.7	13f	1199.5	13f	1176.2	13f	1175.3	13f	1193.4	13f	1089.5	13f	1131.1
14f	1021.9	14f	946.2	14f	1024.1	14f	1131.1	14f	1144.6	14f	1145.9	14f	1133.9	14f	1064.0	14f	1129.1
15f	954.4	15f	932.6	15f	941.1	15f	1086.5	15f	999.9	15f	1103.8	15f	1075.0	15f	987.4	15f	1016.4
16f	923.0	16f	924.3	16f	903.6	16f	986.9	16f	938.6	16f	1015.5	16f	1033.9	16f	954.7	16f	917.5
17f	912.1	17f	741.0	17f	869.5	17f	967.7	17f	917.8	17f	989.3	17f	945.4	17f	947.0	17f	898.8
18f	844.8	18f	713.9	18f	793.6	18f	940.6	18f	889.1	18f	939.5	18f	918.7	18f	872.1	18f	830.8
19f	726.3	19f	584.2	19f	737.1	19f	848.0	19f	832.8	19f	848.0	19f	833.7	19f	826.7	19f	789.3
20f	595.0	20f	529.3	20f	609.8	20f	718.8	20f	610.6	20f	823.5	20f	584.6	20f	718.7	20f	590.2
21f	535.8	21f	432.3	21f	502.0	21f	441.7	21f	445.0	21f	507.3	21f	501.2	21f	622.1	21f	512.4
22f	387.2	22f	423.7	22f	472.1	22f	384.0	22f	411.2	22f	463.7	22f	395.0	22f	544.5	22f	401.7
23f	270.8	23f	317.4	23f	380.7	23f	359.6	23f	359.2	23f	358.8	23f	377.0	23f	413.9	23f	368.5
24f	253.3	24f	296.6	24f	345.4	24f	251.5	24f	249.7	24f	295.0	24f	261.6	24f	378.4	24f	268.0
25f	188.1	25f	247.1	25f	310.4	25f	219.0	25f	239.6	25f	243.9	25f	255.4	25f	319.4	25f	252.0
26f	147.4	26f	213.9	26f	286.8	26f	170.4	26f	209.7	26f	222.1	26f	167.9	26f	266.7	26f	208.6
27f	147.0	27f	178.8	27f	246.9	27f	151.7	27f	180.2	27f	207.6	27f	132.8	27f	249.2	27f	191.8
28f	121.1	28f	174.9	28f	223.2	28f	134.3	28f	139.5	28f	175.3	28f	123.9	28f	210.4	28f	141.2
29f	114.4	29f	134.6	29f	182.1	29f	104.1	29f	119.9	29f	116.5	29f	88.1	29f	189.8	29f	95.7
30f	81.1	30f	116.7	30f	158.0	30f	92.5	30f	96.5	30f	105.8	30f	85.6	30f	131.0	30f	83.4
31f	74.7	31f	106.4	31f	124.8	31f	90.1	31f	86.4	31f	96.1	31f	83.0	31f	124.7	31f	74.5
32f	60.7	32f	85.1	32f	92.9	32f	84.5	32f	74.2	32f	85.3	32f	77.1	32f	90.6	32f	68.5
33f	42.9	33f	80.3	33f	74.5	33f	70.8	33f	69.2	33f	81.7	33f	43.0	33f	76.7	33f	33.3
34f	9.0	34f	71.8	34f/i	71.7	34f	16.6	34f	43.6	34f/i	49.5	34f/i	21.7	34f	64.2	34f/i	25.4
35f/i	46.6	35f	63.8	35f/i	67.4	35f/i	80.5	35f/i	29.8	35f/i	31.3	35f/i	60.8	35f	41.8	35f/i	50.5
36f/i	863.3	36f	264.4	36f/i	333.6	36f/i	350.7	36f/i	445.9	36f/i	817.4	36f/i	550.0	36f/i	818.3	36f/i	652.3

Table S15.

The results of frequency analysis of transition states on CoCuO-Cl surface

TS_1		TS_2		TS_3		TS_4		TS_7		TS_5		TS_6		TS_8		TS_9	
1f	3146.6	1f	3525.4	1f	3685.3	1f	3083.0	1f	3161.5	1f	3078.1	1f	3108.2	1f	3182.2	1f	3204.5
2f	3094.6	2f	3230.9	2f	3157.5	2f	3073.5	2f	3075.4	2f	3063.6	2f	3082.8	2f	3081.2	2f	3084.0
3f	3071.8	3f	3180.6	3f	3074.8	3f	3060.0	3f	3051.8	3f	3007.0	3f	3015.7	3f	3063.7	3f	3073.2
4f	3050.9	4f	3084.4	4f	3068.2	4f	3005.6	4f	3046.6	4f	2999.1	4f	3013.2	4f	3049.6	4f	3065.5
5f	2950.5	5f	3081.4	5f	2791.5	5f	2959.1	5f	3034.3	5f	2942.1	5f	2955.3	5f	2973.6	5f	2984.0
6f	1574.8	6f	3078.9	6f	2241.8	6f	2803.9	6f	2961.8	6f	2355.5	6f	2910.3	6f	2119.6	6f	2968.8
7f	1487.9	7f	1501.1	7f	1614.5	7f	1459.8	7f	1451.1	7f	1464.9	7f	1446.4	7f	1434.1	7f	1448.5
8f	1423.9	8f	1461.1	8f	1400.2	8f	1402.5	8f	1436.4	8f	1411.2	8f	1436.2	8f	1402.6	8f	1433.8
9f	1392.7	9f	1385.0	9f	1280.9	9f	1382.4	9f	1410.7	9f	1393.1	9f	1391.2	9f	1389.7	9f	1412.7
10f	1329.0	10f	1329.3	10f	1266.4	10f	1351.5	10f	1372.0	10f	1330.6	10f	1356.2	10f	1365.2	10f	1364.4
11f	1295.2	11f	1249.0	11f	1254.7	11f	1336.1	11f	1341.6	11f	1250.1	11f	1319.1	11f	1295.5	11f	1339.0
12f	1256.6	12f	1231.5	12f	1154.9	12f	1212.5	12f	1305.1	12f	1207.1	12f	1261.7	12f	1256.7	12f	1243.2
13f	1183.9	13f	1031.6	13f	1086.2	13f	1179.7	13f	1184.2	13f	1168.8	13f	1184.1	13f	1122.4	13f	1168.2
14f	1040.8	14f	977.9	14f	1011.9	14f	1142.2	14f	1141.7	14f	1142.4	14f	1166.7	14f	1046.4	14f	1129.9
15f	977.0	15f	957.8	15f	982.2	15f	1085.0	15f	996.1	15f	1122.6	15f	1124.2	15f	1005.7	15f	1042.0
16f	954.3	16f	926.2	16f	934.2	16f	988.8	16f	931.4	16f	1001.4	16f	1013.5	16f	971.7	16f	906.6
17f	933.9	17f	897.1	17f	876.6	17f	946.9	17f	896.7	17f	954.1	17f	943.2	17f	910.3	17f	887.3
18f	910.6	18f	842.4	18f	788.1	18f	895.4	18f	886.1	18f	907.1	18f	892.9	18f	865.7	18f	837.9
19f	656.9	19f	632.0	19f	751.4	19f	790.4	19f	824.8	19f	851.4	19f	872.2	19f	811.1	19f	815.2
20f	603.0	20f	594.0	20f	611.2	20f	681.5	20f	614.9	20f	795.9	20f	690.9	20f	654.1	20f	568.4
21f	489.6	21f	403.2	21f	452.3	21f	419.9	21f	450.3	21f	462.9	21f	453.8	21f	578.1	21f	418.2
22f	404.9	22f	305.8	22f	434.0	22f	387.3	22f	382.7	22f	450.2	22f	400.9	22f	522.0	22f	408.2
23f	288.4	23f	234.0	23f	393.3	23f	247.3	23f	342.0	23f	276.7	23f	364.8	23f	370.5	23f	350.2
24f	254.9	24f	221.8	24f	334.4	24f	223.5	24f	250.1	24f	244.4	24f	253.1	24f	315.4	24f	309.0
25f	210.9	25f	216.2	25f	266.2	25f	187.8	25f	182.8	25f	236.8	25f	237.7	25f	268.2	25f	258.7
26f	142.0	26f	166.6	26f	259.5	26f	154.0	26f	173.8	26f	203.2	26f	198.6	26f	248.4	26f	210.7
27f	109.0	27f	133.7	27f	193.6	27f	110.6	27f	160.1	27f	177.6	27f	160.5	27f	219.6	27f	186.3
28f	100.8	28f	114.9	28f	132.4	28f	89.3	28f	111.1	28f	133.6	28f	115.8	28f	186.0	28f	156.5
29f	78.7	29f	94.2	29f	119.4	29f	72.1	29f	102.0	29f	117.6	29f	91.8	29f	114.9	29f	122.8
30f	66.8	30f	77.1	30f	104.7	30f	65.4	30f	74.3	30f	81.4	30f	76.0	30f	100.7	30f	76.1
31f	54.3	31f	71.1	31f	78.3	31f	48.5	31f	71.8	31f	71.3	31f	68.2	31f	85.3	31f	67.9
32f	46.6	32f	62.1	32f	68.3	32f	38.4	32f	69.8	32f	68.3	32f	53.1	32f	77.0	32f	63.9
33f	12.2	33f	44.5	33f	61.1	33f/i	29.7	33f	59.6	33f	44.8	33f	35.2	33f	72.6	33f	58.5
34f/i	8.0	34f	32.6	34f	53.3	34f/i	48.5	34f	43.1	34f/i	37.6	34f/i	27.1	34f	63.8	34f	53.9
35f/i	42.0	35f/i	50.8	35f	11.1	35f/i	56.7	35f/i	72.1	35f/i	50.8	35f/i	50.4	35f	45.6	35f	15.2
36f/i	1606.5	35f/i	260.0	36f/i	174.6	36f/i	466.7	36f/i	366.5	36f/i	821.2	36f/i	513.7	36f/i	1208.7	36f/i	629.0

Table S16.

The results of frequency analysis of transition states on LaO surface

TS_1		TS_2		TS_3		TS_4		TS_7		TS_5		TS_6		TS_8		TS_9	
1f	3147.0	1f	3740.5	1f	3705.1	1f	3133.9	1f	3172.1	1f	3072.6	1f	3049.0	1f	3165.2	1f	3189.2
2f	3072.9	2f	3192.8	2f	3157.8	2f	3043.5	2f	3064.0	2f	3035.6	2f	3031.6	2f	3102.8	2f	3074.7
3f	3058.1	3f	3174.8	3f	3073.3	3f	3034.4	3f	3056.7	3f	3024.4	3f	2993.3	3f	3051.4	3f	3060.8
4f	3050.2	4f	3093.5	4f	2978.9	4f	3007.9	4f	3046.3	4f	2961.0	4f	2974.8	4f	3034.1	4f	3037.6
5f	3019.8	5f	3075.6	5f	2845.7	5f	2987.6	5f	3008.4	5f	2895.0	5f	2916.6	5f	2946.9	5f	2954.0
6f	2963.6	6f	3067.4	6f	1632.4	6f	2918.7	6f	2939.6	6f	1665.9	6f	2906.6	6f	2360.3	6f	2946.0
7f	1640.1	7f	1473.7	7f	1433.3	7f	1449.9	7f	1451.0	7f	1555.6	7f	1448.9	7f	1452.1	7f	1452.2
8f	1443.6	8f	1466.7	8f	1399.3	8f	1429.7	8f	1445.8	8f	1438.7	8f	1426.5	8f	1426.8	8f	1440.5
9f	1420.0	9f	1378.0	9f	1345.5	9f	1421.9	9f	1416.3	9f	1432.3	9f	1420.2	9f	1394.7	9f	1399.2
10f	1396.4	10f	1237.8	10f	1275.0	10f	1373.3	10f	1359.6	10f	1352.9	10f	1373.0	10f	1340.5	10f	1351.2
11f	1343.3	11f	1199.6	11f	1265.9	11f	1340.1	11f	1331.9	11f	1342.1	11f	1333.7	11f	1304.6	11f	1322.1
12f	1287.4	12f	1013.2	12f	1138.1	12f	1202.9	12f	1189.0	12f	1290.5	12f	1268.1	12f	1187.9	12f	1226.5
13f	1162.0	13f	968.7	13f	1095.6	13f	1154.3	13f	1146.4	13f	1137.9	13f	1173.4	13f	1044.6	13f	1144.3
14f	1075.9	14f	906.7	14f	1010.3	14f	1112.4	14f	1120.6	14f	1107.1	14f	1162.3	14f	998.8	14f	1138.4
15f	1032.0	15f	786.8	15f	973.8	15f	1011.9	15f	983.8	15f	1047.9	15f	1110.0	15f	938.6	15f	1031.6
16f	999.5	16f	743.6	16f	924.3	16f	961.1	16f	911.0	16f	1014.4	16f	1018.7	16f	891.5	16f	901.0
17f	923.4	17f	547.5	17f	906.7	17f	910.3	17f	886.8	17f	963.0	17f	950.0	17f	803.7	17f	873.7
18f	913.3	18f	530.7	18f	747.8	18f	884.7	18f	835.1	18f	866.1	18f	904.5	18f	744.4	18f	823.7
19f	898.8	19f	498.9	19f	656.2	19f	848.7	19f	647.3	19f	740.8	19f	885.9	19f	615.5	19f	593.6
20f	589.2	20f	411.7	20f	487.0	20f	736.5	20f	502.6	20f	680.8	20f	633.3	20f	519.7	20f	474.2
21f	404.1	21f	338.9	21f	440.0	21f	425.1	21f	476.7	21f	462.5	21f	399.4	21f	468.0	21f	424.8
22f	368.7	22f	299.6	22f	378.1	22f	348.2	22f	398.6	22f	399.0	22f	380.7	22f	371.6	22f	408.6
23f	203.1	23f	282.2	23f	343.8	23f	329.1	23f	327.6	23f	361.7	23f	295.7	23f	359.0	23f	358.2
24f	201.5	24f	183.8	24f	289.8	24f	265.1	24f	244.1	24f	291.2	24f	281.5	24f	302.8	24f	327.5
25f	113.0	25f	176.2	25f	225.6	25f	186.3	25f	221.5	25f	223.8	25f	228.8	25f	207.8	25f	279.8
26f	110.2	26f	164.9	26f	188.9	26f	159.1	26f	175.8	26f	160.1	26f	205.5	26f	188.1	26f	252.7
27f	87.8	27f	59.1	27f	144.4	27f	147.3	27f	163.9	27f	132.3	27f	127.3	27f	156.8	27f	174.6
28f	78.5	28f	53.4	28f	114.7	28f	99.9	28f	123.4	28f	101.6	28f	94.8	28f	114.9	28f	117.6
29f	41.9	29f	47.2	29f	79.9	29f	62.2	29f	91.6	29f	61.2	29f	73.3	29f	93.1	29f	110.9
30f	36.2	30f	36.1	30f	72.1	30f	60.8	30f	51.5	30f	33.8	30f	63.9	30f	74.5	30f	60.6
31f	15.1	31f	32.6	31f	52.0	31f/i	27.5	31f/i	16.1	31f	47.3	31f	49.7	31f	33.9	31f	24.6
32f/i	25.6	32f/i	10.0	32f	42.1	32f/i	52.8	32f/i	51.5	32f/i	5.6	32f/i	30.1	32f/i	19.0	32f/i	42.0
33f/i	669.9	33f/i	183.7	33f/i	1327.8	33f/i	471.3	33f/i	415.3	33f/i	907.7	33f/i	392.5	33f/i	1058.5	33f/i	398.2

Table S17.

The results of frequency analysis of transition states on LaCuO surface

TS_1		TS_2		TS_3		TS_4		TS_7		TS_5		TS_6		TS_8		TS_9	
1f	3156.5	1f	3719.1	1f	3713.4	1f	3136.5	1f	3169.1	1f	3107.2	1f	3061.4	1f	3158.9	1f	3165.6
2f	3104.4	2f	3184.0	2f	3152.4	2f	3048.9	2f	3064.0	2f	3072.8	2f	3042.7	2f	3106.7	2f	3075.5
3f	3065.3	3f	3145.4	3f	3072.1	3f	3048.4	3f	3047.8	3f	2992.0	3f	2996.7	3f	3051.2	3f	3041.9
4f	3062.6	4f	3077.3	4f	2974.0	4f	3028.4	4f	3042.6	4f	2921.3	4f	2980.1	4f	3044.4	4f	3039.5
5f	3014.7	5f	3063.9	5f	2835.3	5f	2988.1	5f	3012.0	5f	2837.3	5f	2923.6	5f	2972.2	5f	3023.7
6f	1541.9	6f	3044.1	6f	1627.1	6f	2917.4	6f	2945.5	6f	2016.0	6f	2896.1	6f	2389.8	6f	2929.7
7f	1434.9	7f	1476.0	7f	1431.8	7f	1455.6	7f	1454.0	7f	1444.5	7f	1452.8	7f	1450.3	7f	1476.1
8f	1416.9	8f	1471.4	8f	1404.1	8f	1425.2	8f	1449.2	8f	1402.9	8f	1432.2	8f	1428.4	8f	1447.0
9f	1375.6	9f	1386.6	9f	1314.1	9f	1415.8	9f	1420.3	9f	1397.1	9f	1415.7	9f	1396.9	9f	1412.3
10f	1260.9	10f	1232.2	10f	1275.0	10f	1365.1	10f	1359.5	10f	1367.1	10f	1376.9	10f	1342.5	10f	1368.3
11f	1198.0	11f	1200.5	11f	1250.6	11f	1341.5	11f	1329.5	11f	1323.8	11f	1332.0	11f	1261.2	11f	1324.8
12f	1086.9	12f	1022.8	12f	1143.9	12f	1199.3	12f	1201.0	12f	1235.5	12f	1255.4	12f	1196.5	12f	1246.8
13f	1082.9	13f	983.4	13f	1095.6	13f	1152.9	13f	1146.6	13f	1111.7	13f	1174.2	13f	1053.3	13f	1168.5
14f	999.1	14f	913.1	14f	1016.3	14f	1096.8	14f	1129.5	14f	1096.6	14f	1163.9	14f	994.3	14f	1145.0
15f	957.9	15f	810.4	15f	981.8	15f	1005.6	15f	985.3	15f	1025.4	15f	1109.6	15f	967.7	15f	1085.9
16f	926.6	16f	750.7	16f	917.4	16f	967.4	16f	916.7	16f	983.7	16f	1033.5	16f	892.4	16f	942.6
17f	911.0	17f	546.3	17f	900.9	17f	902.3	17f	898.2	17f	921.8	17f	943.1	17f	812.1	17f	912.2
18f	836.8	18f	517.8	18f	748.3	18f	875.6	18f	855.2	18f	909.3	18f	905.5	18f	752.0	18f	862.7
19f	653.2	19f	489.3	19f	646.5	19f	852.2	19f	637.2	19f	711.6	19f	880.6	19f	614.4	19f	815.0
20f	621.2	20f	411.3	20f	498.9	20f	709.5	20f	514.6	20f	666.1	20f	692.9	20f	518.0	20f	707.2
21f	464.9	21f	400.1	21f	437.1	21f	431.7	21f	479.8	21f	420.8	21f	389.3	21f	495.9	21f	440.7
22f	364.3	22f	365.2	22f	368.3	22f	365.5	22f	382.6	22f	339.4	22f	364.7	22f	383.3	22f	398.6
23f	286.5	23f	330.3	23f	298.3	23f	318.4	23f	310.8	23f	276.2	23f	313.8	23f	314.8	23f	386.5
24f	263.0	24f	314.0	24f	278.0	24f	252.1	24f	244.3	24f	263.0	24f	270.1	24f	255.0	24f	357.1
25f	228.9	25f	146.0	25f	236.8	25f	186.2	25f	225.3	25f	173.5	25f	205.9	25f	229.3	25f	295.4
26f	183.1	26f	124.9	26f	190.6	26f	161.3	26f	200.9	26f	155.4	26f	173.6	26f	161.4	26f	282.5
27f	154.7	27f	82.3	27f	127.6	27f	128.8	27f	185.0	27f	121.3	27f	119.6	27f	139.3	27f	204.3
28f	130.8	28f	78.9	28f	89.3	28f	88.4	28f	107.6	28f	99.5	28f	102.1	28f	114.4	28f	164.1
29f	96.1	29f	52.4	29f	61.8	29f	70.1	29f	75.9	29f	56.6	29f	74.4	29f	65.8	29f	144.0
30f	66.1	30f	28.3	30f	42.8	30f	43.3	30f	50.4	30f	29.6	30f	42.6	30f	32.9	30f	98.7
31f	52.0	31f/i	47.6	31f	31.9	31f	17.3	31f/i	45.0	31f/i	68.2	31f	16.0	31f/i	11.9	31f	38.5
32f/i	21.6	32f/i	59.5	32f/i	58.1	32f	6.8	32f/i	57.4	32f/i	192.8	32f/i	42.6	32f/i	101.6	32f	33.3
33f/i	1270.7	33f/i	146.3	33f/i	1257.8	33f/i	508.7	33f/i	426.0	33f/i	1044.2	33f/i	564.6	33f/i	1060.0	33f/i	246.4

Table S18.

The results of frequency analysis of transition states on LaO-Cl surface

TS_1		TS_2		TS_3		TS_4		TS_7		TS_5		TS_6		TS_8		TS_9	
1f	3143.7	1f	3739.5	1f	3679.0	1f	3143.2	1f	3165.6	1f	3113.7	1f	3066.1	1f	3182.2	1f	3166.0
2f	3099.5	2f	3206.7	2f	3141.4	2f	3086.0	2f	3095.9	2f	3076.8	2f	3034.5	2f	3081.2	2f	3084.2
3f	3075.6	3f	3162.3	3f	3092.3	3f	3076.9	3f	3073.4	3f	3044.4	3f	3008.5	3f	3063.7	3f	3077.2
4f	3066.7	4f	3079.9	4f	2995.6	4f	3037.2	4f	3057.6	4f	2961.3	4f	2994.2	4f	3049.6	4f	3064.5
5f	2990.3	5f	3061.8	5f	2873.1	5f	3008.4	5f	3031.7	5f	2857.6	5f	2964.2	5f	2973.6	5f	2977.7
6f	1563.9	6f	3017.9	6f	1634.1	6f	2962.5	6f	2990.3	6f	2033.1	6f	2956.4	6f	2119.6	6f	2925.5
7f	1437.4	7f	1485.3	7f	1533.3	7f	1472.0	7f	1454.1	7f	1458.2	7f	1463.7	7f	1434.1	7f	1452.9
8f	1414.5	8f	1469.6	8f	1413.2	8f	1432.8	8f	1450.1	8f	1418.2	8f	1439.6	8f	1402.6	8f	1441.0
9f	1382.8	9f	1383.0	9f	1315.5	9f	1412.3	9f	1431.1	9f	1400.6	9f	1428.6	9f	1389.7	9f	1401.7
10f	1279.2	10f	1239.2	10f	1289.3	10f	1375.1	10f	1367.1	10f	1379.6	10f	1371.8	10f	1365.2	10f	1356.9
11f	1204.9	11f	1206.4	11f	1274.5	11f	1338.4	11f	1333.1	11f	1333.0	11f	1341.3	11f	1295.5	11f	1328.0
12f	1139.3	12f	1020.4	12f	1159.3	12f	1190.6	12f	1209.9	12f	1244.2	12f	1274.0	12f	1256.7	12f	1246.3
13f	1035.7	13f	993.2	13f	1106.7	13f	1163.2	13f	1157.4	13f	1141.0	13f	1183.2	13f	1122.4	13f	1143.6
14f	1021.8	14f	911.5	14f	1023.8	14f	1103.2	14f	1139.4	14f	1107.8	14f	1163.2	14f	1046.4	14f	1108.9
15f	952.5	15f	815.4	15f	1012.3	15f	995.6	15f	986.2	15f	1035.5	15f	1115.9	15f	1005.7	15f	1019.1
16f	941.1	16f	778.5	16f	943.3	16f	959.7	16f	954.8	16f	1002.0	16f	1022.9	16f	971.7	16f	905.9
17f	930.4	17f	550.1	17f	918.3	17f	906.7	17f	921.2	17f	941.7	17f	959.2	17f	910.3	17f	873.5
18f	843.1	18f	529.1	18f	783.3	18f	878.1	18f	891.7	18f	920.1	18f	916.0	18f	865.7	18f	799.6
19f	679.5	19f	500.1	19f	679.8	19f	862.9	19f	664.7	19f	746.7	19f	877.8	19f	811.1	19f	746.4
20f	645.6	20f	412.1	20f	553.5	20f	743.1	20f	519.6	20f	684.6	20f	640.1	20f	654.1	20f	603.2
21f	471.1	21f	360.1	21f	483.9	21f	440.8	21f	484.2	21f	444.1	21f	400.8	21f	578.1	21f	505.7
22f	358.3	22f	318.1	22f	404.3	22f	343.4	22f	397.4	22f	333.5	22f	381.6	22f	522.0	22f	412.3
23f	286.4	23f	291.7	23f	364.9	23f	323.8	23f	310.1	23f	293.4	23f	304.2	23f	370.5	23f	346.2
24f	260.5	24f	222.7	24f	268.9	24f	260.7	24f	266.7	24f	275.2	24f	272.4	24f	315.4	24f	312.5
25f	217.7	25f	170.7	25f	240.6	25f	216.7	25f	261.0	25f	204.1	25f	237.9	25f	268.2	25f	282.3
26f	179.7	26f	151.3	26f	197.7	26f	170.9	26f	221.2	26f	173.0	26f	183.0	26f	248.4	26f	265.4
27f	176.7	27f	129.5	27f	180.6	27f	168.4	27f	197.9	27f	165.0	27f	159.2	27f	219.6	27f	172.5
28f	148.1	28f	111.8	28f	165.5	28f	132.9	28f	168.2	28f	158.8	28f	153.1	28f	186.0	28f	156.0
29f	114.5	29f	83.5	29f	135.9	29f	106.8	29f	110.9	29f	143.4	29f	146.5	29f	114.9	29f	143.8
30f	104.7	30f	72.5	30f	96.5	30f	85.7	30f	98.1	30f	112.8	30f	109.8	30f	100.7	30f	104.5
31f	62.3	31f	82.6	31f	87.8	31f	62.9	31f	84.1	31f	88.1	31f	96.4	31f	85.3	31f	86.9
32f	55.2	32f	55.6	32f	68.5	32f	48.4	32f	78.0	32f	78.5	32f	87.8	32f	77.0	32f	76.9
33f	26.3	33f	50.5	33f	63.1	33f	36.4	33f	76.6	33f	8.8	33f	63.5	33f	72.6	33f	63.6
34f	9.8	34f	31.4	34f	31.9	34f/i	74.8	34f	60.2	34f/i	27.8	34f	48.7	34f	63.8	34f	40.8
35f/i	71.9	35f/i	24.5	35f/i	59.5	35f/i	81.9	35f/i	42.4	35f/i	54.7	35f/i	79.0	35f	45.6	35f/i	57.9
36f/i	1398.4	35f/i	200.5	36f/i	1007.0	36f/i	527.3	36f/i	434.7	36f/i	838.4	36f/i	413.6	36f/i	1208.7	36f/i	349.7

Table S19.

The results of frequency analysis of transition states on LaCuO-Cl surface

TS_1		TS_2		TS_3		TS_4		TS_7		TS_5		TS_6		TS_8		TS_9	
1f	3152.6	1f	3729.9	1f	3643.8	1f	3130.5	1f	3167.4	1f	3102.0	1f	3066.6	1f	3164.2	1f	3140.0
2f	3101.8	2f	3189.9	2f	3157.4	2f	3061.8	2f	3071.2	2f	3066.5	2f	3049.6	2f	3122.6	2f	3126.3
3f	3067.2	3f	3150.6	3f	3071.7	3f	3049.8	3f	3055.8	3f	3008.1	3f	3005.8	3f	3063.0	3f	3073.4
4f	3058.6	4f	3081.7	4f	2998.0	4f	3026.4	4f	3035.5	4f	2919.2	4f	2987.9	4f	3047.5	4f	3072.1
5f	3012.4	5f	3068.6	5f	2851.1	5f	2968.0	5f	3019.2	5f	2835.9	5f	2932.6	5f	3009.5	5f	3024.6
6f	1544.4	6f	3052.8	6f	1634.1	6f	2934.1	6f	2954.9	6f	2030.4	6f	2903.5	6f	2320.3	6f	2866.2
7f	1435.3	7f	1474.0	7f	1551.1	7f	1468.9	7f	1450.3	7f	1455.0	7f	1457.4	7f	1447.2	7f	1453.3
8f	1424.4	8f	1466.0	8f	1406.4	8f	1431.4	8f	1444.1	8f	1407.4	8f	1427.4	8f	1435.5	8f	1439.8
9f	1373.4	9f	1381.9	9f	1305.5	9f	1412.0	9f	1425.1	9f	1397.5	9f	1417.8	9f	1401.9	9f	1403.6
10f	1261.8	10f	1231.0	10f	1280.3	10f	1373.0	10f	1362.4	10f	1369.9	10f	1373.3	10f	1355.1	10f	1356.0
11f	1195.6	11f	1197.1	11f	1263.5	11f	1347.0	11f	1333.4	11f	1322.3	11f	1331.9	11f	1302.3	11f	1270.2
12f	1097.2	12f	1014.3	12f	1142.3	12f	1196.3	12f	1202.4	12f	1238.0	12f	1263.1	12f	1209.9	12f	1257.9
13f	1068.7	13f	984.4	13f	1097.8	13f	1165.9	13f	1148.3	13f	1116.0	13f	1170.3	13f	1057.8	13f	1136.1
14f	998.8	14f	905.3	14f	1018.0	14f	1091.1	14f	1141.6	14f	1092.9	14f	1164.0	14f	1006.1	14f	1109.2
15f	954.7	15f	811.2	15f	966.9	15f	989.1	15f	988.1	15f	1017.6	15f	1110.7	15f	969.6	15f	996.6
16f	939.2	16f	763.0	16f	926.7	16f	957.3	16f	946.0	16f	995.9	16f	1025.9	16f	896.0	16f	904.4
17f	914.6	17f	557.3	17f	895.3	17f	895.3	17f	916.6	17f	926.3	17f	942.6	17f	816.1	17f	892.5
18f	822.7	18f	544.2	18f	769.4	18f	875.8	18f	886.8	18f	900.9	18f	904.8	18f	757.4	18f	839.0
19f	643.5	19f	523.0	19f	653.5	19f	764.1	19f	653.7	19f	725.3	19f	884.0	19f	630.0	19f	778.1
20f	621.4	20f	408.5	20f	569.5	20f	636.8	20f	522.1	20f	675.0	20f	657.3	20f	552.9	20f	722.1
21f	464.5	21f	356.4	21f	468.0	21f	418.0	21f	492.2	21f	424.0	21f	403.3	21f	476.5	21f	544.7
22f	362.3	22f	316.2	22f	418.3	22f	358.3	22f	394.4	22f	338.0	22f	384.2	22f	380.8	22f	394.6
23f	282.2	23f	295.4	23f	375.5	23f	336.2	23f	302.2	23f	285.4	23f	309.8	23f	339.3	23f	373.6
24f	266.0	24f	184.4	24f	288.6	24f	270.1	24f	239.0	24f	270.6	24f	279.5	24f	310.1	24f	333.5
25f	212.3	25f	181.5	25f	247.0	25f	212.3	25f	218.8	25f	201.9	25f	224.6	25f	218.3	25f	250.5
26f	188.7	26f	157.3	26f	197.1	26f	175.8	26f	202.3	26f	166.6	26f	173.0	26f	192.4	26f	193.3
27f	172.4	27f	145.2	27f	150.1	27f	142.3	27f	189.1	27f	146.9	27f	171.1	27f	169.0	27f	171.8
28f	141.6	28f	115.7	28f	129.3	28f	115.0	28f	178.9	28f	142.5	28f	121.6	28f	165.5	28f	165.3
29f	116.7	29f	89.1	29f	88.6	29f	101.6	29f	114.9	29f	120.5	29f	118.8	29f	141.4	29f	147.2
30f	104.5	30f	76.0	30f	74.4	30f	77.6	30f	113.9	30f	96.3	30f	104.4	30f	123.5	30f	120.2
31f	83.7	31f	51.2	31f	61.0	31f	65.7	31f	86.0	31f	51.1	31f	87.0	31f	99.5	31f	84.4
32f	80.7	32f	48.7	32f	51.3	32f	48.9	32f	80.8	32f	47.5	32f	75.0	32f	85.1	32f	58.2
33f	65.0	33f	46.7	33f	32.6	33f	24.3	33f	49.2	33f	28.0	33f	53.1	33f	74.1	33f	52.4
34f	25.4	34f	27.5	34f	16.8	34f	58.2	34f	29.3	34f/i	34.7	34f	46.7	34f	45.8	34f	15.9
35f/i	12.2	35f	26.6	35f/i	38.9	35f/i	23.3	35f/i	56.7	35f/i	86.8	35f/i	34.1	35f/i	67.3	35f	42.8
36f/i	1247.1	35f/i	155.0	36f/i	832.1	36f/i	499.4	36f/i	425.4	36f/i	1080.2	36f/i	472.1	36f/i	1236.2	36f/i	303.8