#### **Supporting Information**

# Nano Si-doped Ruthenium Oxide Particles from Caged Precursors for High-Performance Acidic Oxygen Evolution

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### **S1** Materials and Methods

#### S1-1: Materials and Equipments

All materials were used as received without further purification, unless otherwise noted. Ethanol was dried with Mg turnings.

All manipulations were carried out in air atmosphere, unless otherwise noted. The high resolution transmission electron microscopy (HRTEM) experiments were recorded on a Hitachi 7650 electron microscope. The scanning electron microscopy (SEM) and energy dispersive X-ray spectrometry (EDS) were recorded on a Jeol JSM-7500F field emission scanning electron microscope. The IR spectra were recorded with KBr pellets on a Bruker EQUINOX 55 FT-spectrometer in the range of 4000–500 cm<sup>-1</sup>. Powder X-ray diffraction (PXRD) patterns were recorded on Bruker D8 Advance analytical diffractometers for Cu K = radiation ( $\lambda = 1.5406$  Å). ICP-OES measurement was performed using Optima-7000 DV spectrometer. Raman spectroscopy was conducted on a Jobin Yvon LabRAM HR 800 instrument with a 532 nm excitation laser at a power of around 0.8 mW.

Data reduction, data analysis, and EXAFS fitting were performed with the Athena and Artemis software packages. The energy calibration of the sample was conducted through a standard Ru foil, which was simultaneously measured as a reference. For EXAFS modeling, EXAFS of the Ru foil is fitted, and the obtained amplitude reduction factor  $S_0^2$  value (0.890) was set in the EXAFS analysis to determine the coordination numbers (CNs) in the Ru-O/Si scattering path. For Wavelet Transform analysis, the  $\chi(k)$  exported from Athena was imported into the Hama Fortran code. The parameters were listed as follow: R range, 1 - 3.5 Å, k range, 0 - 13.0 Å<sup>-1</sup> for sample (0 - 13.0 Å<sup>-1</sup> for Ru foil and RuO<sub>2</sub>); k weight, 2; and Morlet function with  $\kappa = 10$ ,  $\sigma = 1$  was used as the mother wavelet to provide the overall distribution.

#### **S1-2: Materials Preparation**

Metal sources RuCl<sub>3</sub>·xH<sub>2</sub>O and sodium alginate were purchased from Aladdin. Nafion<sup>®</sup> perfluorinated resin solution containing 5% Nafion<sup>®</sup> was purchased from Sigma-Aldrich. Ultrapure water with resistivity > 18 M $\Omega$ ·cm<sup>-1</sup> was used.

#### Preparation of RuO<sub>x</sub>/C

The RuCl<sub>3</sub> (56 mg) was dissolved in absolute ethanol (8 mL) and stirred for 30 min to give a transparent red solution. To the ultra-dry DMF (72 mL) was added commercial acetylene black (96 mg), and the ultrasonic dispersing of this suspension was performed for 30 min. A 20 mL vial was charged with the above-mentioned RuCl<sub>3</sub> solution (1 mL) and acetylene black dispersion (12 mL). The vial was sealed under air and placed in drying oven at 85 °C for 72 h. The mixture was then cooled to room temperature and dried under vacuum, and the residual black powder was transferred to the muffle furnace at 450 °C for 6 h. The RuO<sub>x</sub>/C was obtained as a black powder.

#### Preparation of Si-RuOx@C

The RuCl<sub>3</sub> (56 mg) was dissolved in absolute ethanol (8 mL) and stirred for 30 min to give a transparent red solution. As an organic cage for which we have reported the synthetic method,<sup>[1]</sup> COP1-T (96 mg) was dissolved in ultra-dry DMF (12 mL) and stirred at 150 mL round bottom flask for 30 min. A 20 mL vial was charged with the above-mentioned RuCl<sub>3</sub> solution (1 mL), COP1-T solution (12 mL), and triethylamine (12  $\mu$ L) (the Si/Ru mass ratio is 1 : 8.5). The vial was sealed under air and placed in drying oven at 85 °C for 72 h. Then the reaction flask was cooled to room temperature, dried, and then transferred to a muffle furnace. In order to explore the influence of temperature on OER performance, we adopted the same method to prepare catalysts at different temperatures at 150 °C, 250 °C, 350 °C, 450 °C and 550 °C respectively.

#### Preparation of RuO<sub>x</sub>/L1



Figure S1. The structure of L1.

The hexaphenylbenzene carboxylic acid molecule (L1) was prepared according to our previous report. The RuCl<sub>3</sub> (56 mg) was dissolved in absolute ethanol (8 mL) and stirred for 30 min to give a transparent red solution. To an ultra-dry DMF solution (72 mL) of (96mg) L1<sup>[1]</sup> and the solution was stirred for 30 min. A 20 mL vial was charged with the abovementioned RuCl<sub>3</sub> solution (1 mL), the COP1-T solution with silane (12 mL), and triethylamine (12  $\mu$ L). The vial was sealed under air and placed in drying oven at 85 °C for 72 h. Then the reaction flask was cooled to room temperature, dried, and then transferred to a muffle furnace at 450 °C for 6 h to give RuO<sub>x</sub>@L1 as a black powder.

#### Preparation of Si3-RuOx@C

The RuCl<sub>3</sub> (56 mg) was dissolved in absolute ethanol (8 mL) and stirred for 30 min to give a transparent red solution. To an ultra-dry DMF solution (72 mL) of COP1-T (96 mg) was added chloro(dimethylphenyl)silane (6.58 mg) and the solution was stirred for 30 min. A 20 mL vial was charged with the above-mentioned RuCl<sub>3</sub> solution (1 mL), the COP1-T solution with silane (12 mL), and triethylamine (12  $\mu$ L) (the Si/Ru mass ratio is 2 : 8.5). The vial was sealed under air and placed in drying oven at 85 °C for 72 h. Then the reaction flask was cooled to room temperature, dried, and then transferred to a muffle furnace at 450 °C for 6 h to give Si<sub>3</sub>-RuO<sub>x</sub>@C as a black powder.

#### Preparation of Si<sub>4</sub>-RuO<sub>x</sub>@C

The RuCl<sub>3</sub> (56 mg) was dissolved in absolute ethanol (8 mL) and stirred for 30 min to give a transparent red solution. To an ultra-dry DMF solution (72 mL) of COP1-T (96 mg) was added chloro(dimethylphenyl)silane (13.16 mg) and stirred for 30 min. A 20 mL vial was charged with the above-mentioned RuCl<sub>3</sub> solution (1 mL), the COP1-T solution with silane (12 mL), and triethylamine (12  $\mu$ L) (the Si/Ru mass ratio is 3 : 8.5). The vial was sealed under air and placed in drying oven at 85 °C for 72 h. Then the reaction flask was cooled to room temperature, dried, and then transferred to a muffle furnace at 450 °C for 6 h to give Si<sub>4</sub>-RuO<sub>x</sub>@C as a black powder.

#### **S1-3: Material Characterization**

#### **Electrochemical experiments**

Cyclic voltammetry (CV) measurements were carried out in a standard one-compartment cell equipped with a carbon rob counter electrode [Ag/AgCl (3 M KCl)], a reference electrode (Hg/HgO), and a glassy carbon (GC) working electrode. The measurements were performed in deionized water with 0.5 M H<sub>2</sub>SO<sub>4</sub>, 1 M KOH and 1 M phosphate buffered saline (PBS) as the supporting electrolyte. The data is collected and processed by the Shanghai electrochemical analyzer (CHI760e) at 25 °C. The linear sweep voltammetry (LSV) for OER were recorded in 0.5 M H<sub>2</sub>SO<sub>4</sub> at the potential range from 1.0 – 1.6 V (vs.RHE). The LSVs for HER were recorded in 0.5 M H<sub>2</sub>SO<sub>4</sub> at the potential range of -2 - 0 V (vs. RHE). The electrochemical surface area was determined by a double layer capacitance (C<sub>dl</sub>) method, in which the doublelayer charging currents were measured in  $0.5 \text{ M H}_2\text{SO}_4$  at the potential range from 0.1 - 0.2 Vand at the scanning rates range from 10 to 100 mV·s<sup>-1</sup>. Cyclic voltammetry curves were measured at different scan rates (20 mV·s<sup>-1</sup>, 40 mV·s<sup>-1</sup>, 60 mV·s<sup>-1</sup>, 80 mV·s<sup>-1</sup> 100 mV·s<sup>-1</sup>). In the overall water splitting (OWS), two Si-RuO<sub>x</sub>@C electrodes acted as the negative electrode for HER and the positive electrode for OER, respectively. The LSV was recorded at a scan rate of 5 mV·s<sup>-1</sup>. For the benchmark control, commercial Pt/C was used as the negative electrode and commercial RuO<sub>2</sub> as the positive electrode.

For the preparation of working electrode, Si-RuO<sub>x</sub>@C catalyst (5 mg) was dispersed in the mixture of Nafion<sup>®</sup> (50  $\mu$ L, 5 wt.%) solution and ethanol (450  $\mu$ L). Then a homogenous catalyst ink was obtained by ultrasonic dispersion. The resulting ink (31  $\mu$ L) was pipetted onto a glassy carbon disk (0.196 cm<sup>2</sup>). The mass loading of catalyst is 1.6 mg·cm<sup>-2</sup>. For comparison, working electrodes of commercial RuO<sub>2</sub> and RuO<sub>x</sub>@C with mass loading of 1.6 mg·cm<sup>-2</sup> were also prepared by the same procedure.

For the durability test of the catalyst supported on carbon fiber, the Si-RuO<sub>x</sub>@C catalyst (3 mg) was dispersed in 0.5 mL mixture of ethanol (0.25 mL) and water (0.25 mL) with Nafion<sup>®</sup> solution (10  $\mu$ L, 5 wt.%, DuPont) to form homogeneous ink by ultrasonic dispersion. Then the ink was added dropwise onto the surface of carbon paper with 1 cm<sup>2</sup> by using a micropipette and dried at room temperature. The final loading for all catalysts is 1.6 mg·cm<sup>-2</sup> on carbon paper.

All potentials were referenced to the reversible hydrogen electrode (RHE) by the equations as follows (Eq.1 and Eq. 2):

$$E(RHE) = E(Ag/AgCl, 3 M KCl - filled) + 0.059 pH + 0.197$$
 (Eq. 1)

E(RHE) = E(Hg/Hg0, 1 M KOH - filled) + 0.059 pH + 0.098 (Eq. 2)

All electrochemical data were not subjected to IR compensation.

#### DFT calculations

Vienna Ab-initio Simulation Package (VASP) was used for all calculations with Revised Perdew-Burke-Ernzerhof (RPBE) functional for the exchange-correlation term and the projector augmented wave method<sup>[2-9]</sup>.

The cutoff energies for all calculations were set to 520 eV. To consider the impact of van der Waals interactions between graphene and RuO<sub>2</sub> surface, the dispersion interaction corrected DFT (DFT-D<sub>2</sub>) method was introduced in the structure optimization.<sup>[10]</sup> All structures were fully relaxed to the ground state and spin-polarization was considered in all calculations. The convergences of energy and force were set to  $1 \times 10^{-5}$  eV and 0.01 eV·Å<sup>-1</sup>, respectively. The vacuum space value is set to 20 Å to separate the interaction between neighboring slabs. As for OER, the free energies of the intermediates at 298.15 K were obtained by the following

equation (Eq. 3):

 $\Delta G = \Delta E + \Delta ZPE - T\Delta S + eU$  (Eq. 3)

In this equation,  $\Delta E$  is the binding energy of adsorption species HO\*, O\* and HOO\*,  $\Delta ZPE$ ,  $\Delta S$  and U are the zeropoint energy changes, entropy changes and applied potentials, respectively. Furthermore, the energy barrier ( $\eta$ ) was calculated by the following equation (Eq. 4):

 $\eta = (\Delta G_{OOH*} - \Delta G_{O*} - 1.23)/e$  (Eq. 4)

In this equation, the asterisk represents active site, and 1.23 V stands for the equilibrium potential under the standard condition.

For pure RuO<sub>2</sub> catalyst, the RuO<sub>2</sub> (110) surface with  $4 \times 5$  supercell was chosen as the structure. For Si introduced RuO<sub>2</sub> (110), one of the surface Ru was replaced by Si atom. In order to minimize the influence of lattice mismatch, we have carefully chosen the supercells for RuO<sub>2</sub> and the models are listed in S3-1, S3-2, S3-3.

### **S2** Figures and Tables



Figure S2. The DLS of COP1-T and COP1-T@NP.



**Figure S3.** a) K-edge EXAFS spectrum of K-space Si-RuO<sub>x</sub>@C, Ru foil and RuO<sub>2</sub>. b) K-edge EXAFS fitting curve of K-space Si-RuO<sub>x</sub>@C. c) EXAFS fitting curve of RuO<sub>2</sub>. d) EXAFS fitting curve of Ru foil. e) and f) WT-EXAFS spectrum of Ru foil and RuO<sub>2</sub>, respectively.

Sample	Shell	$CN^a$	R (Å) <sup>b</sup>	$\sigma^2 (\text{\AA}^2)^c$	$\Delta E_0 ({ m eV})^d$	R factor
Ru foil	Ru-Ru	12*	$2.68\pm0.01$	$0.0044 \pm 0.0003$	$5.7\pm1.0$	0.0046
	Ru-O	$5.8\pm0.6$	$1.98\pm0.01$	$0.0033 \pm 0.0007$		
RuO <sub>2</sub>	Ru-Ru	$3.5\pm0.7$	$3.12\pm0.01$	$0.0047 \pm 0.0009$	$\textbf{-0.2}\pm1.2$	0.0057
	Ru-Ru	$10.1\pm2.0$	$3.56\pm0.01$	$0.0047 \pm 0.0009$		
	Ru-O	$2.7\pm0.2$	$2.01\pm0.01$	$0.0007 \pm 0.0004$		
Ru	Ru-Si	$1.4\pm0.3$	$2.35\pm0.01$	$0.0022 \pm 0.0009$	$\textbf{-13.5}\pm0.8$	0.0104
	Ru-O-Si	$3.8\pm1.2$	$2.84\pm0.01$	$0.0067 \pm 0.0022$		

**Table S1.** EXAFS fitting parameters at the Ru K-edge for various samples  $(S_0^2 = 0.790)$ 

<sup>*a*</sup>*CN*, coordination number; <sup>*b*</sup>*R*, distance between absorber and backscatter atoms; <sup>*c*</sup> $\sigma^2$ , Debye-Waller factor to account for both thermal and structural disorders; <sup>*d*</sup> $\Delta E_0$ , inner potential correction; *R* factor indicates the

goodness of the fit.  $S_0^2$  was fixed to 0.790, according to the experimental EXAFS fit of M foil by fixing CN as the known crystallographic value. Fitting range:  $3.0 \le k$  (/Å)  $\le 17.8$  and  $2.0 \le R$  (Å)  $\le 3.0$  (Ru foil);  $3.0 \le k$  (/Å)  $\le 13.0$  and  $1.0 \le R$  (Å)  $\le 3.8$  (RuO<sub>2</sub>);  $3.0 \le k$  (/Å)  $\le 14.0$  and  $1.0 \le R$  (Å)  $\le 3.0$  (Ru). A reasonable range of EXAFS fitting parameters:  $0.700 < S_0^2 < 1.000$ ; CN > 0;  $\sigma^2 > 0$  Å<sup>2</sup>;  $\Delta E_0 < 15$  eV; R factor < 0.02.



**Figure S4.** XRD diagram of Si-RuO<sub>x</sub>@C calcined at different temperatures. Two tests were done for the samples of Si-RuO<sub>x</sub>@C, indicating that the peaks around 30° (in the red box) are attributed to unindentified impurities introduced during the sample preparation other than from the catalysts. 450 °C-1 represents the first test, whereas 450 °C-2 represents the second test.



Figure S5. a) LSV of Si-RuO<sub>x</sub>@C in 1 M KOH (pH = 14). b) LSV of Si-RuO<sub>x</sub>@C in 1 M PBS (pH = 6.8).

		acidic m	iedia.		
Catalyst	Electrolyte solution	Overpotential (mV)	Stability	Loading amount (mg·cm <sup>-2</sup> )	Ref.
Si-RuO <sub>x</sub> @C	0.5 M H <sub>2</sub> SO <sub>4</sub>	$\eta_{10} = 220$	100 h (10 mA·cm <sup>-2</sup> )	0.017 (Ru)	This work
RuO <sub>x</sub> @C	$0.5 \text{ M} \text{H}_2 \text{SO}_4$	$\eta_{10} = 260$	_	1.6	This work
$RuO_2$	$0.5 \text{ M} \text{H}_2\text{SO}_4$	$\eta_{10} = 300$	_	1.6	This work
6H-SrIrO <sub>3</sub>	$0.5 \text{ M} \text{H}_2\text{SO}_4$	$\eta_{10} = 248$	$30 \text{ h} (10 \text{ mA} \cdot \text{cm}^{-2})$	0.90	[11]
IrO <sub>2</sub> -NPs	$0.5 \mathrm{~M~H_2SO_4}$	$\eta_{10} = 297$	4.0 h (20 mA·cm <sup>-2</sup> )	0.20 (IrO <sub>2</sub> )	[12]
Ru@IrO <sub>x</sub>	0.05 M	$\eta_{10} = 282$	$2 h (10 mA \cdot cm^{-2})$	0.05	[13]
	$H_2SO_4$				
IrNi-NCs	0.1 M HClO <sub>4</sub>	_	$2 h (5 mA \cdot cm^{-2})$	0.0125 (Ir)	[14]
Li-IrO <sub>x</sub>	$0.5 \mathrm{~M~H_2SO_4}$	$\eta_{10}=300$	10 h (10 mA·cm <sup>-2</sup> )	0.05	[15]
$Ba_4PrIr_3O_{12}$	0.1 M HClO <sub>4</sub>	$\eta_{10} = 278$	10 h (10 mA·cm <sup>-2</sup> )	0.56	[16]
IrO <sub>2</sub> -RuO <sub>2</sub> @Ru	0.5 M H <sub>2</sub> SO <sub>4</sub>	$\eta_{10} = 281$	2 h (1.6 V)	0.100	[17]
Co-IrCuONC	0.1 M HClO <sub>4</sub>	$\eta_{10} = 293$	_	0.020 (Ir)	[18]
W <sub>0.57</sub> Ir <sub>0.43</sub> O <sub>3</sub> δ	1.0 M H <sub>2</sub> SO <sub>4</sub>	$\eta_{10} = 370$	0.55 h (10 mA·cm <sup>-2</sup> )	-	[19]
Ir-W-B alloy	$0.5 \mathrm{~M~H_2SO_4}$	$\eta_{10} = 291$	800 h (100 mA·cm <sup>-2</sup> )	0.079 (Ir)	[20]
IrO <sub>x</sub> /SrIrO <sub>3</sub>	$0.5 \mathrm{~M~H_2SO_4}$	$\eta_{10} = 290$	30.0 h (10 mA·cm <sup>-2</sup> )	_	[21]
Pt/IrO <sub>2</sub>	0.5 M H <sub>2</sub> SO <sub>4</sub>	$\eta_{10} = 348$	_	0.38	[22]
Ir <sub>3</sub> Cu	0.1 M HClO <sub>4</sub>	$\eta_{10} = 298$	$12.0 \text{ h} (5 \text{ mA} \cdot \text{cm}^{-2})$	_	[23]
Pd-Ir-Pd	0.1 M HClO <sub>4</sub>	$\eta_{10} = 372$	_	0.017	[24]
IrO <sub>x</sub> -Ni	$0.5 \mathrm{~M~H_2SO_4}$	$\eta_{10} = 290$	$100 \text{ h} (2 \text{ mA} \cdot \text{cm}^{-2})$	0.13 (Ir)	[25]

Table S2. Comparison of OER performance for Si-RuO<sub>x</sub>@C with some benchmark Ir-based oxides in



Figure S6. a) LSV test of Si-RuO<sub>x</sub>@C at different temperatures in 0.5 M  $H_2SO_4$ . b) Mass activity and overpotential.



**Figure S7.** (a) The comparison between the OER performance of  $RuO_x@L1$  and  $Si-RuO_x@C$ . (b) $Si-RuO_x@C$  OER test with different Si contents. The  $RuO_x@C$  sample contains no Si. The Si/Ru mass ratio of Si-RuO\_x@C is 1 : 8.5; the Si/Ru mass ratio of Si<sub>3</sub>-RuO<sub>x</sub>@C is 2 : 8.5; the Si/Ru mass ratio of Si<sub>4</sub>-RuO<sub>x</sub>@C is 3 : 8.5.



**Figure S8.** The Si-RuO<sub>x</sub>@C of CV stability test. a) the LSV of before and after CV test. b) During the CV test, the potential changes with the number of scanning cycles at 10 mA·cm<sup>-2</sup>.



**Figure S9.** HRTEM diagrams of Si-RuO<sub>x</sub>@C after CV test. a) to d) The data were collected on various scales.



Figure S10. SEM and mapping diagrams of Si-RuO<sub>x</sub>@C after CV test.



Figure S11. EDS diagram of Si-RuO<sub>x</sub>@C after CV test.



Figure S12. The XPS of Si-RuO<sub>x</sub>@C comparison before and after CV stability test.



**Figure S13.** a) HER performance test of Si-RuO<sub>x</sub>@C in 0.5 M H<sub>2</sub>SO<sub>4</sub>. b) OWS LSV curves without iR compensation. c) Stability test of Si-RuO<sub>x</sub>@C||Si-RuO<sub>x</sub>@C and Pt/C||RuO<sub>2</sub> for OWS at  $j = 10 \text{ mA} \cdot \text{cm}^{-2}$ .



Figure S14. Si-RuO<sub>x</sub>@C DFT calculation models. a) ①: Ru-intra-Si-1, ②: Ru-intra-Si-2 and ③: Ru-

intra-Si. b) ①: Ru-O<sub>5</sub>-Si and ②: Ru-O<sub>5</sub>-Si-1. c) ①: Ru-O<sub>4</sub>-Si and ②: Ru-O<sub>4</sub>-Si-1.



**Figure S15.** a), c) and e)The four-electron mechanism of Ru-intra-Si-1, Ru-intra-Si-2 and Ru-intra-Si toward acidic OER. b), d) and f) The Gibbs free energy diagrams for Ru-intra-Si-1, Ru-intra-Si-2 and Ru-intra-Si.



**Figure S16.** a) and c) The four-electron mechanism of Ru-O<sub>5</sub>-Si and Ru-O<sub>5</sub>-Si-1 toward acidic OER. b) and d) The Gibbs free energy diagrams for Ru-O<sub>5</sub>-Si and Ru-O<sub>5</sub>-Si-1.



**Figure S17.** a) and c) The four-electron mechanism of Ru-O<sub>4</sub>-Si and Ru-O<sub>4</sub>-Si-1 toward acidic OER. b) and d) The Gibbs free energy diagrams for Ru-O<sub>4</sub>-Si and Ru-O<sub>4</sub>-Si-1.



**Figure S18**. Si-RuO<sub>x</sub>@C partial charge of different Si replacing Ru. a) and b) Ru-intra-Si. c) and d) Ru-O<sub>5</sub>-Si. e) and f) Ru-O<sub>4</sub>-Si.



**Figure S19.** a) The TDOS of Ru-intra-Si, Ru-O<sub>4</sub>-Si and Ru-O<sub>5</sub>-Si. b) The PDOS of Ru for Ru-intra-Si, Ru-O<sub>4</sub>-Si and Ru-O<sub>5</sub>-Si.



Figure S20. Ru-intra-Si, Ru-O<sub>5</sub>-Si and Ru-O<sub>4</sub>-Si of DOS. a) TDOS. b) The PDOS of O. c) The PDOS of Si.



**Figure S21**. Differential charge density at the interface Ru centers between  $RuO_x$  and Si. Yellow and cyan contours represent electron accumulation and depletion, respectively. a) and b) Ru-intra-Si. c) and d) Ru-O<sub>5</sub>-Si. e) and f) Ru-O<sub>4</sub>-Si.

## **S3 Modeling**

## S3-1: Optimized structure information of Ru-intra-Si

1.00000000000000			
12.7746000290000001 0.0	000000000000000000000000000000000000000	00 0.000000000000000	000
0.000000000000000 9.2	77000427200000	0.0000000000000000000000000000000000000	000
0.0000000000000000000000000000000000000	000000000000000000000000000000000000000	0 16 963 3998870999	996
	000000000000000000000000000000000000000	50 10.9055990070999	<i>))</i> 0
24 48 1			
24 40 I Selective dynamics			
Dive et			
	212000125450	0 7010445002050004	<b></b>
0.1342831815/99521 0.1628	312000135450	0.7818445823058006	
0.3/35100099999968 0.1664	1/0001999999/0	0.5962/003699999965	FFF
0.3/2226/396062425 -0.0102	2535843915347	0.7867733247599732	
0.125000000000000 0.0000	30000000024	0.5932999589999994	FFF
0.6151273522371494 0.1543	296480820611	0.7831056702361591	ТТТ
0.8764899709999980 0.1664	799990000034	0.5962700369999965	FFF
0.8768372787994272 0.0348	3654914897338	0.7870651665594197	ТТТ
0.6250000089999972 0.9970	399810000004	0.5892799820000008	FFF
0.1135891350840483 0.5068	961112355548	0.7792799461987966	ТТТ
0.3738000029999995 0.5004	300120000025	0.5964099669999996	FFF
0.3764651477502776 0.3420	0004936633695	0.7884725023699457	ТТТ
0.12500000000000 0.3334	5999099999980	0.5935599740000015	FFF
0.5783068299798798 0.4207	515394938743	0.7936355803733015	ТТТ
0.8762000159999985 0.5004	300120000025	0.5964099669999996	FFF
0.8705870934837782 0.3209	281259087828	0.7866336927374172	ТТТ
0.6249599949999975 0.3483	400140000015	0.5698599580000021	FFF
0.1136180126109520 0.8412	687926101394	0.7863901263718303	ТТТ
0 3747499750000003 0 8332	499970000029	0 5963500370000006	FFF
0.3654959296133010 0.6813	805820010193	0 7876636618756205	ттт
0.125000000000000 0.6664	0000020010195	0.5935500240000025	FFF
0.6277478964790687 0.8581	204785675300	0.57555500240000025	ттт
0.875240060000022 0.8333	204785075500	0.5063300740000028	FFF
0.8832033680654582 0.6064	1015506083015	0.3903399740000028	ттт
0.625010012000007 0.6602	50016000002	0.7847080297077980	
0.0250100150000007 0.0095	000000000000000000000000000000000000000	0.383313330333333	
	000000000000000000000000000000000000000	0.4/81000210000050	г г г Е Е Е
0.3/301999/99999991 0.9999	0994099999990	0.5214400409999987	ггг
0.3/256819160/3/63 -0.0019	9345338929563	0.6/455/9088408045	
0.1215310853584145 0.0020	1868636469///	0./1104991/2831852	
0.4652659481/05139 0.156/	25544/361046	0.800/449385538519	
0.222590001000004 0.1665	599900000032	0.5956399849999983	FFF
0.2813089392419789 0.1698	5165932469486	0./991493694134381	
0.02/4100020000034 0.1665	599900000032	0.5956399849999983	FFF
0.6250000089999972 0.0000	000000000000000000000000000000000000000	0.4781000210000030	FFF
0.8749799460000034 0.9999	0994699999990	0.5214400469999987	FFF
0.8789135636527921 0.0044	358/08909386	0.6/4/854604419632	TTT
0.6226952913473185 -0.0030	0406160887296	0.7074019833986194	ТТТ
0.9882991243337250 0.1812	2367865952139	0.8034747790062265	ТТТ
0.7243999479999985 0.1631	000040000004	0.5959699929999971	FFF
0.7616261867693804 0.1673	422933722294	0.8020370038709858	ТТТ
0.5256100369999999 0.1631	100020000034	0.5959699929999971	FFF
0.12500000000000 0.3333	300010000002	0.4781000210000030	FFF
0.3752099920000020 0.3333	200040000008	0.5215099850000016	FFF
0.3738208107310216 0.3335	559614392560	0.6753457926175831	ТТТ
0.1241602038022797 0.3365	691804628109	0.7130770842450546	ТТТ
0.4564313717483368 0.5206	801581956382	0.8252791375378478	ТТТ
0.2225600089999986 0.5000	000000000000000000000000000000000000000	0.5956299770000015	FFF
0.2658107512145878 0.5099	929793276344	0.8008396678637614	ТТТ
0.0274400010000022 0.5000	000000000000000	0.5956299770000015	FFF
0.6250000089999972 0.3333	300010000002	0.4781000210000030	FFF
0.8747900259999994 0 3333	20004000008	0.5215099850000016	FFF
0.8742808159432325 0.3323	559572490103	0.6735688151838055	ТТТ

	0.6147829650365318	0.3159609670978287	0.7052675702059231	Т	Т	Т
	0.9592665977767432	0.5049320428723399	0.7974772155147819	Т	Т	Т
	0.7248399590000005	0.5034899520000025	0.5953099760000029	F	F	F
	0.7416804564833999	0.4447585761271655	0.8118095055024830	Т	Т	Т
	0.5251600229999980	0.5034899520000025	0.5953099760000029	F	F	F
	0.1250000000000000	0.6666700250000019	0.4781000210000030	F	F	F
	0.3749199989999994	0.6666999910000015	0.5214800199999985	F	F	F
	0.3743285690969987	0.6679103437629353	0.6759802127540949	Т	Т	Т
	0.1256729053942614	0.6738288487007330	0.7120097496862310	Т	Т	Т
	0.4796754728314281	0.8375359694525135	0.8032528187741271	Т	Т	Т
	0.2226600070000018	0.8333699639999992	0.5956700059999989	F	F	F
	0.2628742179436348	0.8356637695039987	0.8055809688895385	Т	Т	Т
	0.0273300010000028	0.8333699639999992	0.5956700059999989	F	F	F
	0.6250000089999972	0.6666700250000019	0.4781000210000030	F	F	F
	0.8750799820000026	0.6666999910000015	0.5214700120000018	F	F	F
	0.8744831615105020	0.6667287207926200	0.6744544065788082	Т	Т	Т
	0.6417712702791911	0.6671708376484693	0.7086586086206157	Т	Т	Т
	0.9733707277346458	0.8713243114150064	0.8192275756671368	Т	Т	Т
	0.7227799579999967	0.8338199709999969	0.5952800109999998	F	F	F
	0.7833586040433997	0.8679872665232095	0.7995540767002247	Т	Т	Т
	0.5272200240000018	0.8338299939999985	0.5952700039999996	F	F	F
_	0.7080078500632053	0.6147402138675931	0.7881257913253804	Т	Т	Т

S3-2: Optimized structure information of Ru-O5-Si

1.000000000000
12.774600029000001  0.0000000000000  0.00000000000
0.00000000000000  9.2770004272000008  0.00000000000000000000000000000
0.00000000000000  0.0000000000000  16.9633998870999996
Ru O Si
47 84 1
Selective dynamics
Direct
0.7517578884392704 0.3370715187757228 0.7790003421703239 T T T
0.2482420925607315 0.6629284552242750 0.7790003421703239 T T T
0.7517578884392704 0.6629284552242750 0.7790003421703239 T T T
0.2482420925607315 0.3370715187757228 0.7790003421703239 T T T
0.7499999810000020 0.3333300010000002 0.4037599839999970 F F F
0.250000000000000 0.6666699729999976 0.4037599839999970 F F F
0.7499999810000020 0.6666699729999976 0.4037599839999970 F F F
0.250000000000000 0.3333300010000002 0.4037599839999970 F F F
0.7499999810000020 0.1666699989999998 0.2170400090000015 F F F
0.250000000000000 0.8333300270000024 0.2170400090000015 F F F
0.7499999810000020 0.8333300270000024 0.2170400090000015 F F F
0.250000000000000 0.1666699989999998 0.2170400090000015 F F F
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0.2502724121515704 0.8329421955824224 0.5926908230143353 T T T
0.7497275688484313 0.8329421955824224 0.5926908230143353 T T T
0.2502724121515704 0.1670578304175795 0.5926908230143353 T T T
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0.00000000000000 0.66666699729999976 0.22187001199999966 F F F
-0.00000000000000 0.3338396095315111 0.5971997258638047 T T T
-0.000000000000000 0.6661603644684867 0.5971997258638047 T T T
-0.00000000000000 0.1485520226106694 0.7833149515707718 T T T
-0.00000000000000 0.8514480033893328 0.7833149515707718 T T T
0.000000000000000 0.1666699989999998 0.40695999999999980 F F F
0.000000000000000 0.8333300270000024 0.40695999999999980 F F F
0.500000000000000 0.3333300010000002 0.2218700119999966 F F F
0.500000000000000 0.6666699729999976 0.2218700119999966 F F F
0.500000000000000 0.3321299875528147 0.5945801371658349 T T T
0.500000000000000 0.6678699864471833 0.5945801371658349 T T T
0.500000000000000 0.1774443916022496 0.7819821445056887 T T T
0.500000000000000 0.8225556343977524 0.7819821445056887 T T T
0.50000000000000 0.166669998999998 0.4069599999999980 F F F

0.749999981000020 0.5000000000000 0.217040009000015 F F F 0.2500000000000000 0.5000000000000 0.592599704314044 T T T 0.00000000000000 0.5000000000000 0.592599704314044 T T T 0.00000000000000 0.5000000000000 0.46959999999980 F F F 0.50000000000000 0.5000000000000 0.469599999999980 F F F 0.50000000000000 0.00000000000 0.2218700119999966 F F F 0.00000000000000 0.00000000000 0.7785449988207338 T T T 0.2500341100200566 0.0000000000000 0.7785449988207338 T T T 0.2500000000000000 0.000000000000 0.40637599839999970 F F F 0.500000000000000 0.000000000000 0.2218700119999966 F F F 0.500000000000000 0.000000000000 0.2218700119999966 F F F 0.500000000000000 0.000000000000 0.24187100021000030 F F F 0.2500000000000000 0.1666699989999998 0.478100021000030 F F F 0.250000000000000 0.1666699898999998 0.478100021000030 F F F 0.25000000000000 0.1666699889399998 0.478100021000030 F F F 0.25000000000000 0.16666599889399998 0.478100021000030 F F F 0.25000000000000 0.16666599889399998 0.37076306977255792 T T T 0.252452982735935 0.16930592339853 0.7076306977255792 T T T 0.252452982735935 0.16930592339853 0.7076306977255792 T T T 0.252452982735935 0.1693059239853 0.7076306977255792 T T T 0.252452982735935 0.16930592399976 0.19933997000013 F F F 0.25000000000000 0.333330027000024 0.329430012000031 F F F 0.25000000000000 0.3333300270000024 0.329430012000031 F F F 0.250000000000000 0.33333001000002 0.399330012000031 F F F 0.25000000000000 0.33333001000002 0.19933997000013 F F F 0.25000000000000 0.33333001000002 0.19933997000013 F F F 0.9073799989909970 0.33333001000002 0.40380013000015 F F F 0.9737999981000020 0.33333001000002 0.40380013000015 F F F 0.9737999989000030 0.33333001000002 0.40380013000015 F F F 0.973799989909975 0.66669972999976 0.19933997000013 F F F 0.90232596800573 0.572379711017227 0.7952759605276652 T T T 0.42646999199970 0.33333001000002 0.40380013000015 F F F 0.97380026999999 0.033333001000002 0.403800013000015 F F F 0.97379988939347 0.666669972999976 0.19933997000013 F F F 0.90730396959	0.50000000000000 0.8333300270000024	0 40695999999999980	F	F	F
0.2500000000000000 0.5000000000000 0.217040009000015 F F F 0.74998806792795764 0.500000000000000 0.5925997043141044 T T T 0.00000000000000 0.5000000000000 0.5925997043141044 T T T 0.00000000000000 0.500000000000 0.406959999999980 F F F 0.50000000000000 0.500000000000 0.406959999999980 F F F 0.50000000000000 0.00000000000 0.21875011952619509483 T T T 0.260034110020366 - 0.0000000000000 0.5785449988207538 T T T 0.260034110020366 - 0.0000000000000 0.7785449988207538 T T T 0.260034110020366 - 0.00000000000000 0.437599839999970 F F F 0.50000000000000 0.000000000000 0.437599839999970 F F F 0.50000000000000 0.666669989899998 0.4781000210000030 F F F 0.250000000000000 0.666699898999998 0.4781000210000030 F F F 0.250000000000000 0.666699893999998 0.4781000210000030 F F F 0.245429827359355 0.8306943337601069 0.7076306977255792 T T T 0.747469982640663 0.1693056922398953 0.7076306977255792 T T T 0.747946982640663 0.83036943337601069 0.7076306977255792 T T T 0.2524529827359355 0.8306943337601069 0.7076306977255792 T T T 0.2454529827359355 0.8306943337601069 0.7076306977255792 T T T 0.245045982640663 0.333330027000024 0.329430012000031 F F F 0.250000000000000 0.1666699729999976 0.19933997000013 F F F 0.250000000000000 0.333330001000002 0.19939997000013 F F F 0.350309989000030 0.33333001000002 0.199399997000013 F F F 0.350309989000030 0.366669725999976 0.403800013000015 F F F 0.303039989000033 0.33333001000002 0.19939997000013 F F F 0.303039989000033 0.33333001000002 0.19939997000013 F F F 0.304696999992 0.666669729999976 0.403800013000015 F F F 0.303339001000002 0.199939970 0.433800013000015 F F F 0.3042620469999992 0.33333001000002 0.19939997000013 F F F 0.30489760288082344 0.666669729999976 0.403800013000015 F F F 0.304897692898999975 0.33333001000002 0.199339997000013 F F F 0.30489760288082344 0.666669	0.7400000000000000000000000000000000000	0.2170400090000015	F	F	F
0.290000000000000 0.500000000000 0.5925997043414044 T T T 0.200100000000000 0.5000000000000 0.5925997043414044 T T T T 0.00000000000000 0.5000000000000 0.466959999999980 F F F F 0.50000000000000 0.5000000000000 0.466959999999980 F F F F 0.00000000000000 0.0000000000		0.217040000000015	Г	г Б	Г
0.498806/92/95/0744 0.500000000000000 0.5925997043414044 T T T 0.20000000000000 0.5000000000000 0.592597043414044 T T T 0.00000000000000 0.5000000000000 0.466959999999980 F F F 0.00000000000000 0.500000000000 0.2218700119999966 F F F 0.000000000000000 0.0000000000 0.5215702619509438 T T T 0.260034110020056 - 0.00000000000000 0.7785449988207538 T T T 0.260034110020056 - 0.00000000000000 0.251451176875905 T T T 0.250000000000000 0.000000000000 0.259451176875905 T T T 0.7399999810000020 0.666669982999998 0.4781000210000030 F F F 0.250000000000000 0.833330027000024 0.4781000210000030 F F F 0.250000000000000 0.66669989999998 0.4781000210000030 F F F 0.747546982640663 0.1693056922398953 0.7076306977255792 T T T 0.747546982640663 0.1693056922398958 0.37076306977255792 T T T 0.747546982640663 0.1693056922398958 0.37076306977255792 T T T 0.747546982640663 0.166659989999998 0.3294300120000031 F F F 0.25000000000000 0.666669972999998 0.3294300120000031 F F F 0.25000000000000 0.6666699729999976 0.199339970000013 F F F 0.25000000000000 0.6666699729999976 0.199339970000013 F F F 0.350309989000000 0.6666697297999976 0.199339970000013 F F F 0.350309989000003 0.6666697297999976 0.4038000130000015 F F F 0.9026200469999992 0.333330010000002 0.199339970000013 F F F 0.9026200469999992 0.666669729999976 0.403800013000015 F F F 0.9026200469999992 0.666669729999976 0.403800013000015 F F F 0.9026200469999992 0.666669729999976 0.403800013000015 F F F 0.4847602880823441 0.3333774200473976 0.5942538258308109 T T T 0.402619973000002 0.6666699729999976 0.403800013000015 F F F 0.49469001000033 0.6666699729999976 0.403800013000015 F F F 0.404576141		0.21/0400090000015	F	Г Т	Г Т
0.2501193017204256 0.500000000000000 0.592597043414044 T T T T 0.000000000000000 0.5000000000000 0.469559999999980 F F F F 0.50000000000000 0.5000000000000 0.469559999999980 F F F F 0.00000000000000 0.0000000000	0./498806/92/95/64 0.5000000000000000	0.5925997043414044	Т	Т	1
-0.00000000000000 0.5000000000000 0.785843462254439 T T T 0.000000000000000 0.5000000000000 0.221870011999966 F F F 0.00000000000000 0.000000000000 0.221870011999966 F F F 0.260034110020566 -0.00000000000000 0.785449988207538 T T T 0.260034110020566 -0.00000000000000 0.4037599839999970 F F F 0.250000000000000 0.00000000000 0.4037599839999970 F F F 0.250000000000000 0.000000000000 0.221870011999966 F F F 0.50000000000000 0.000000000000 0.221870011999966 F F F 0.50000000000000 0.000000000000 0.596451176875955 T T T 0.749999981000020 0.166669998999998 0.4781000210000030 F F F 0.2500000000000000 0.166669998999998 0.4781000210000030 F F F 0.2500000000000000 0.166669989899998 0.4781000210000030 F F F 0.749999981000020 0.833330027000024 0.4781000210000030 F F F 0.749598240663 0.1693056922398953 0.7076306977255792 T T T 0.74546982640663 0.1693056922398953 0.7076306977255792 T T T 0.25245282735355 0.166669989899998 0.3294300120000031 F F F 0.749999981000020 0.8333300270000024 0.329430012000031 F F F 0.7499999810000020 0.833330027000024 0.329430012000031 F F F 0.2500000000000000 0.166669998999998 0.329430012000031 F F F 0.250000000000000 0.1666699972999976 0.199939970000013 F F F 0.53030998000003 0.666669972999976 0.1999399970000013 F F F 0.350309989000003 0.666669972999976 0.1999399970000013 F F F 0.04960010999970 0.33333001000002 0.403800013000015 F F F 0.9026200469999992 0.33333001000002 0.403800013000015 F F F 0.9026200469999992 0.666669972999976 0.1993399970000013 F F F 0.9026200469999992 0.636669972999976 0.1993399970000013 F F F 0.9026200469999992 0.666669972999976 0.199339970000013 F F F 0.9026200469999992 0.6666699729999976 0.199339970000013 F F F 0.902	0.2501193017204256 0.500000000000000	0.5925997043414044	Т	Т	Т
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0.0973799989999975         0.6666699729999976         0.403800013000015         F         F           0.9026200469999992         0.66666997299999976         0.4038000130000015         F         F           0.0973799989999975         0.3333300010000002         0.1999399970000013         F         F           0.8503099520000035         0.63333300010000002         0.1999399970000013         F         F           0.1496900010000033         0.6666699729999976         0.1999399970000013         F         F           0.1496900010000033         0.3333300010000002         0.1999399970000013         F         F           0.1496900010000033         0.327620202982748         0.7952759605276652         T         T           0.9023325965800573         0.6723797710017227         0.7952759605276652         T         T           0.9023325965800573         0.327620202982748         0.7952759605276652         T         T           0.47692880823441         0.666622539526001         0.5942538258308109         T         T           0.4577692880823441         0.6666251839654673         0.5925437536630022         T         T           0.4515024576415435         0.3337327900345408         0.5925437536630022         T         T           0.4026199730000002         0.333300010	0.9026200469999992 0.3333300010000002	0.4038000130000015	F	F	F
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.507380026000002 0.5555500010000002	0.403800013000013	₁ F	F	F
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.37/30002077777778 0.0000077/27797970	0.4020000120000015	r E	r E	r E
0.59/3800269999998       0.3333300010000002       0.4038000130000015       F       F       F         0.5924298979933527       0.3573329926029064       0.7930339695772228       T       T       T         0.4075701020066476       0.6426669813970916       0.7930339695772228       T       T       T         0.5924298979933527       0.6426669813970916       0.7930339695772228       T       T       T         0.4075701020066476       0.3573329926029064       0.7930339695772228       T       T       T         -0.00000000000000       0.1676280167416447       0.5213295915977543       T       T       T         -0.0000000000000000       0.8323720092583574       0.5213295915977543       T       T       T         0.00000000000000000       0.1666699989999998       0.2897300019999989       F       F       F         0.0000000000000000000000000000000       0.1651042207749199       0.66956283963666933       T       T       T         -0.00000000000000000000000000000000000	0.4020199730000002 0.6666699729999976	0.4038000130000015	F T	F	r T
0.5924298979933527       0.3573329926029064       0.7930339695772228       T       T       T         0.4075701020066476       0.6426669813970916       0.7930339695772228       T       T       T         0.5924298979933527       0.6426669813970916       0.7930339695772228       T       T       T         0.4075701020066476       0.3573329926029064       0.7930339695772228       T       T       T         0.4075701020066476       0.3573329926029064       0.7930339695772228       T       T       T         -0.000000000000000       0.1676280167416447       0.5213295915977543       T       T       T         -0.0000000000000000       0.8323720092583574       0.5213295915977543       T       T       T         0.000000000000000000000000000000       0.1666699989999998       0.2897300019999989       F       F       F         0.00000000000000000000000000000000000	0.59/3800269999998 0.3333300010000002	0.4038000130000015	F	F	F
0.4075701020066476       0.6426669813970916       0.7930339695772228       T       T       T         0.5924298979933527       0.6426669813970916       0.7930339695772228       T       T       T         0.4075701020066476       0.3573329926029064       0.7930339695772228       T       T       T         -0.000000000000000       0.1676280167416447       0.5213295915977543       T       T       T         -0.0000000000000000       0.8323720092583574       0.5213295915977543       T       T       T         0.0000000000000000       0.1666699989999998       0.2897300019999989       F       F       F         0.000000000000000000000       0.1651042207749199       0.6695628396366933       T       T       T         -0.0000000000000000000000000000000       0.8348958052250823       0.6695628396366933       T       T       T         -0.00000000000000000000000000000000000	0.5924298979933527 0.3573329926029064	0.7930339695772228	Т	Т	Т
0.5924298979933527       0.6426669813970916       0.7930339695772228       T       T       T         0.4075701020066476       0.3573329926029064       0.7930339695772228       T       T       T         -0.00000000000000000       0.1676280167416447       0.5213295915977543       T       T       T         -0.000000000000000000       0.8323720092583574       0.5213295915977543       T       T       T         0.00000000000000000       0.166669998999998       0.2897300019999989       F       F       F         0.00000000000000000       0.1651042207749199       0.6695628396366933       T       T       T         -0.000000000000000000000000000000       0.8348958052250823       0.6695628396366933       T       T       T         0.500000000000000000000000000000000000	0.4075701020066476 0.6426669813970916	0.7930339695772228	Т	Т	Т
0.4075701020066476 0.3573329926029064 0.7930339695772228 T T T -0.000000000000000 0.1676280167416447 0.5213295915977543 T T T -0.000000000000000 0.8323720092583574 0.5213295915977543 T T T 0.0000000000000000 0.1666699989999998 0.2897300019999989 F F F 0.000000000000000 0.833330027000024 0.2897300019999989 F F F -0.000000000000000 0.1651042207749199 0.6695628396366933 T T T -0.000000000000000 0.8348958052250823 0.6695628396366933 T T T 0.500000000000000 0.1665159013736313 0.5210515827438966 T T T	0.5924298979933527 0.6426669813970916	0.7930339695772228	Т	Т	Т
-0.000000000000000 0.1676280167416447 0.5213295915977543 T T T -0.0000000000000000 0.8323720092583574 0.5213295915977543 T T T 0.0000000000000000 0.1666699989999998 0.2897300019999989 F F F 0.0000000000000000 0.8333300270000024 0.2897300019999989 F F F -0.000000000000000 0.1651042207749199 0.6695628396366933 T T T -0.000000000000000 0.8348958052250823 0.6695628396366933 T T T 0.5000000000000000 0.1665159013736313 0.5210515827438966 T T T	0.4075701020066476 0.3573329926029064	0.7930339695772228	Т	Т	Т
-0.00000000000000000000000000000000000		0 52132050150775/2	т	Ť	Ť
-0.00000000000000000000000000000000000	-0.00000000000000000000000000000000000	0.5215255715777545	т	т	т
0.000000000000000000000000000000000000		0.32132333137//343	Г	T E	т Б
0.00000000000000000000000000000000000	0.0000000000000000000000000000000000000	0.289/300019999989	r -	r T	r T
-0.00000000000000 0.1651042207749199 0.6695628396366933 T T T -0.000000000000000 0.8348958052250823 0.6695628396366933 T T T 0.500000000000000 0.1665159013736313 0.5210515827438966 T T T	0.0000000000000 0.8333300270000024	0.289/300019999989	F	F	F
-0.00000000000000 0.8348958052250823 0.6695628396366933 T T T 0.50000000000000 0.1665159013736313 0.5210515827438966 T T T	-0.00000000000000 0.1651042207749199	0.6695628396366933	Т	Т	Т
0.50000000000000 0.1665159013736313 0.5210515827438966 T T T	-0.00000000000000 0.8348958052250823	0.6695628396366933	Т	Т	Т
	0.50000000000000 0.1665159013736313	0.5210515827438966	Т	Т	Т

	0.500000000000000000	0.8334841246263709	0.5210515827438966	Т	Т	Т	
	0.50000000000000000	0.1666699989999998	0.2897300019999989	F	F	F	
	0.50000000000000000	0.8333300270000024	0.2897300019999989	F	F	F	
	0.50000000000000000	0.1675940650026730	0.6693126168676233	Т	Т	Т	
	0.50000000000000000	0.8324059609973292	0.6693126168676233	Т	Т	Т	
	0.7499999810000020	0.50000000000000000	0.4781000210000030	F	F	F	
	0.25000000000000000	0.5000000000000000	0.4781000210000030	F	F	F	
	0.7505498125503971	0.50000000000000000	0.7060986351417008	Т	Т	Т	
	0.2494501684496051	0.50000000000000000	0.7060986351417008	Т	Т	Т	
	0.7499999810000020	0.5000000000000000	0.3294300120000031	F	F	F	
	0.25000000000000000	0.50000000000000000	0.3294300120000031	F	F	F	
	-0.00000000000000000	0.50000000000000000	0.5216275286663410	Т	Т	Т	
	0.00000000000000000	0.50000000000000000	0.2897300019999989	F	F	F	
	-0.00000000000000000	0.50000000000000000	0.6723543007363273	Т	Т	Т	
	0.50000000000000000	0.50000000000000000	0.5207804307720092	Т	Т	Т	
	0.50000000000000000	0.5000000000000000	0.2897300019999989	F	F	F	
	0.50000000000000000	0.50000000000000000	0.6730902711559907	Т	Т	Т	
	0.6496900109999970	0.00000000000000000000000000000000000	0.1999399970000013	F	F	F	
	0.3503099890000030	0.00000000000000000	0.1999399970000013	F	F	F	
	0.9026200469999992	0.00000000000000000	0.4038000130000015	F	F	F	
	0.0973799989999975	0.00000000000000000000000000000000000	0.4038000130000015	F	F	F	
	0.8503099520000035	0.00000000000000000	0.1999399970000013	F	F	F	
	0.1496900010000033	0.00000000000000000000000000000000000	0.1999399970000013	F	F	F	
	0.1123211844455559	-0.0000000000000000	0.7978848781477749	Т	Т	Т	
	0.8876788435544393	-0.00000000000000000000000000000000000	0.7978848781477749	Т	Т	Т	
	0.8474262396188776	-0.00000000000000000000000000000000000	0.5936588805486446	Т	Т	Т	
	0.1525737703811232	-0.00000000000000000000000000000000000	0.5936588805486446	Т	Т	Т	
	0.6527290171771454	-0.00000000000000000000000000000000000	0.5937790945835016	Т	Т	Т	
	0.3472709458228549	-0.00000000000000000000000000000000000	0.5937790945835016	Т	Т	Т	
	0.4026199730000002	0.00000000000000000	0.4038000130000015	F	F	F	
	0.5973800269999998	0.00000000000000000000000000000000000	0.4038000130000015	F	F	F	
	0.5925869279306872	-0.00000000000000000000000000000000000	0.7894511713617683	Т	Т	Т	
	0.4074130720693127	-0.00000000000000000000000000000000000	0.7894511713617683	Т	Т	Т	
_	0.50000000000000000	0.50000000000000000	0.7714616566735302	Т	Т	Т	

## S3-3: Optimized structure information of Ru-O4-Si

1.0000000000000				
12.774600029000001 0.00000000000000 0.000000000000	000	0		
0.00000000000000 9.2770004272000008 0.0000000000000	000	)		
0.00000000000000 0.0000000000000 16.9633998870999	999	6		
Ru O Si				
47 84 1				
Selective dynamics				
Direct				
0.25000000000000 0.1666699989999998 0.2218700119999966	F	F	F	
0.7499999810000020 0.8333300270000024 0.2218700119999966	F	F	F	
0.25000000000000 0.8333300270000024 0.2218700119999966	F	F	F	
0.7499999810000020 0.1666699989999998 0.2218700119999966	F	F	F	
0.2499568608285129 0.1669259042513238 0.5972289587431097	Т	Т	Т	
0.7500431201714891 0.8330741217486783 0.5972289587431097	Т	Т	Т	
0.2499568608285129 0.8330741217486783 0.5972289587431097	Т	Т	Т	
0.7500431201714891 0.1669259042513238 0.5972289587431097	Т	Т	Т	
0.2566621685951537 0.3390863227773888 0.7837982009170242	Т	Т	Т	
$0.7433378124048484 \ 0.6609136512226090 \ 0.7837982009170242$	Т	Т	Т	
0.2566621685951537 0.6609136512226090 0.7837982009170242	Т	Т	Т	
0.7433378124048484 0.3390863227773888 0.7837982009170242	Т	Т	Т	
0.25000000000000 0.3333300010000002 0.40695999999999980	F	F	F	
0.7499999810000020 0.66666699729999976 0.4069599999999980	F	F	F	
0.25000000000000 0.6666699729999976 0.4069599999999980	F	F	F	
0.7499999810000020 0.3333300010000002 0.40695999999999980	F	F	F	
0.00000000000000 0.1757037605856138 0.7764364290733806	Т	Т	Т	
0.00000000000000 0.8242962654143884 0.7764364290733806	Т	Т	Т	
0.00000000000000 0.1666699989999998 0.4037599839999970	F	F	F	

0.0000000000000000	0.8333300270000024	0.4037599839999970	F	F	F
0.0000000000000000	0.3333300010000002	0.2170400090000015	F	F	F
0.00000000000000000	0.6666699729999976	0.2170400090000015	F	F	F
0.00000000000000000	0.3342104419386361	0.5919421655950339	Т	Т	Т
0.00000000000000000	0.6657895320613618	0.5919421655950339	Т	Т	Т
0.00000000000000000	0.000000000000000000	0.2170400090000015	F	F	F
0.0000000000000000000000000000000000000	-0.000000000000000000000000000000000000	0 5932469272328562	т	т	T
0.0000000000000000000000000000000000000		0.783112067/065126	т	т	т
0.2400707204030247		0.7821120674065126	т	т	т
0.7519252525945771	-0.000000000000000000000000000000000000	0.7831120074903120	I E	T E	I E
0.23000000000000000	0.0000000000000000000000000000000000000	0.40093999999999980	Г	Г	Г
0.7499999810000020	0.00000000000000000	0.40695999999999980	r T	r T	F T
0.50000000000000000	0.1483134486312015	0.7811361306326695	T	T	T
0.50000000000000000	0.8516865773688007	0.7811361306326695	Т	Т	Т
0.50000000000000000	0.1666699989999998	0.4037599839999970	F	F	F
0.50000000000000000	0.8333300270000024	0.4037599839999970	F	F	F
0.5000000000000000	0.3333300010000002	0.2170400090000015	F	F	F
0.50000000000000000	0.6666699729999976	0.2170400090000015	F	F	F
0.50000000000000000	0.3336248670415082	0.5906561618012344	Т	Т	Т
0.50000000000000000	0.6663751069584896	0.5906561618012344	Т	Т	Т
0 50000000000000000	0.0000000000000000000000000000000000000	0 2170400090000015	F	F	F
0.5000000000000000000000000000000000000	-0.000000000000000000000000000000000000	0.5910102827566550	Т	Т	Т
0.2500000000000000000000000000000000000	0.5000000000000000000000000000000000000	0.221870011000066	F	F	F
0.2300000000000000000000000000000000000	0.5000000000000000000000000000000000000	0.2218700119999900	Г	Г	Г Г
0.7499999810000020	0.5000000000000000000000000000000000000	0.2218/001199999900	Г	г	г
0.250//84450102363	0.50000000000000000	0.596/9548044334//	I	I	I
0.7492215359897655	0.50000000000000000	0.5967954804433477	Т	Т	Т
0.00000000000000000	0.50000000000000000	0.7817506355009595	Т	Т	Т
0.0000000000000000	0.50000000000000000	0.4037599839999970	F	F	F
0.50000000000000000	0.5000000000000000	0.4037599839999970	F	F	F
0.8996900289999985	0.1666699989999998	0.1999399970000013	F	F	F
0.1003099989999967	0.8333300270000024	0.1999399970000013	F	F	F
0.8996900289999985	0.8333300270000024	0.1999399970000013	F	F	F
0 1003099989999967	0 1666699989999998	0 1999399970000013	F	F	F
0.1526200010000025	0.1666600080000008	0.4038000130000015	F	F	F
0.1520200010000025	0.100007770000077	0.402800012000015	Г	Г Б	Г Г
0.04/30000099999903	0.8353500270000024	0.4038000130000015	Г	Г Е	Г Е
0.1526200010000025	0.85555002/0000024	0.4038000130000015	Г Г	F	Г Г
0.84/3800089999983	0.1666699989999998	0.4038000130000015	r T	F	F
0.3473800089999983	0.1666699989999998	0.4038000130000015	F	F	F
0.6526199540000022	0.8333300270000024	0.4038000130000015	F	F	F
0.3473800089999983	0.8333300270000024	0.4038000130000015	F	F	F
0.6526199540000022	0.1666699989999998	0.4038000130000015	F	F	F
0.3494724859699377	0.1644762000100082	0.7931391718475365	Т	Т	Т
0.6505275140300625	0.8355238259899940	0.7931391718475365	Т	Т	Т
0.3494724859699377	0.8355238259899940	0.7931391718475365	Т	Т	Т
0.6505275140300625	0 1644762000100082	0 7931391718475365	т	Т	T
0.0070182074761305	0.1670096773419704	0 5948030866229357	т	т	т
0.0000102074701505	0.1070070775417704	0.5048030866220357	т	т	т
0.902901/4032303/3	0.0329903400300310	0.5946050600229557	т Т	т Т	і т
0.09/01829/4/01595	0.8529905480580518	0.3948030806229337	I T	I T	I T
0.902981/4852385/3	0.10/0090//3419/04	0.3948030806229357	I T	I T	I T
0.1520984211523480	0.1//1689652103/99	0./906133315693840	1	1	1
0.8479015318476585	0.8228310607896224	0.7906133315693840	Т	Т	Т
0.1520984211523480	0.8228310607896224	0.7906133315693840	Т	Т	Т
0.8479015318476585	0.1771689652103799	0.7906133315693840	Т	Т	Т
0.3996899919999990	0.1666699989999998	0.1999399970000013	F	F	F
0.6003099710000015	0.8333300270000024	0.1999399970000013	F	F	F
0.3996899919999990	0.8333300270000024	0.1999399970000013	F	F	F
0.6003099710000015	0.1666699989999998	0.1999399970000013	F	F	F
0.5969609365541597	0.1679439654070300	0.5945437011316416	Ť	Ť	- T
0.403039063///58/02	0.8320560605020721	0 5945437011316/16	Ť	Ť	Ť
0.50606002655/11507	0.8320500005929721	0.50/5/27011216/16	т	т	т Т
0.0202002200224109/	0.0320300003323/21	0.5745457011510410	т	т	т Т
0.4030390034438403	0.10/94390340/0300	0.394343/011310410	I T	I T	1 T
0.2498318/101/5/52	0.3332461/469/6630	0.521//886125018//	1	1	1
0.7501681099824268	0.666/53/993023349	0.5217/88612501877	Т	Т	1
0.2498318710175752	0.6667537993023349	0.5217788612501877	Т	Т	Т
0.7501681099824268	0.3332461746976630	0.5217788612501877	Т	Т	Т
0.25000000000000000	0.3333300010000002	0.2897300019999989	F	F	F
0.7499999810000020	0.6666699729999976	0.2897300019999989	F	F	F
0.25000000000000000	0.6666699729999976	0.2897300019999989	F	F	F

0.7499999810000020	0.3333300010000002	0.2897300019999989	F	F	F
0.2520983765308236	0.3337346535338390	0.6705706034786839	Т	Т	Т
0.7479016044691783	0.6662653204661587	0.6705706034786839	Т	Т	Т
0.2520983765308236	0.6662653204661587	0.6705706034786839	Т	Т	Т
0.7479016044691783	0.3337346535338390	0.6705706034786839	Т	Т	Т
0.00000000000000000	0.3333300010000002	0.4781000210000030	F	F	F
0.000000000000000000	0.6666699729999976	0.4781000210000030	F	F	F
0.00000000000000000	0.3386109315502260	0.7078760861548659	Т	Т	T
0.00000000000000000	0.6613890424497719	0.7078760861548659	Т	Т	T
0.00000000000000000	0.3333300010000002	0.3294300120000031	F	F	F
0.00000000000000000	0.6666699729999976	0.3294300120000031	F	F	F
0.0000000000000000000000000000000000000	0.000000000000000000	0.4781000210000030	F	F	F
0.0000000000000000000000000000000000000	-0.000000000000000000000000000000000000	0 7109396910077961	Т	Т	Т
0.00000000000000000	0.0000000000000000000000000000000000000	0 3294300120000031	F	F	F
0 2498341775782878	-0.000000000000000000000000000000000000	0.5220623287819242	Т	Т	Т
0.7501658034217145	-0.000000000000000000000000000000000000	0.5220623287819242	Ť	т	T
0.2500000000000000000	0.0000000000000000000000000000000000000	0 2897300019999989	F	F	F
0.2300000000000000000000000000000000000	0.0000000000000000000000000000000000000	0.2897300019999989	F	F	F
0.2493650306382748		0.6707220445050501	т	т	т Т
0.7506340503617260	0.0000000000000000000000000000000000000	0.6707220445050501	т	т	T T
0.7500549505017209	0.3333300010000000000000	0.0707229443930391	F	т Б	I E
0.5000000000000000000000000000000000000	0.5555500010000002	0.4781000210000030	Г	Г	r E
0.5000000000000000000000000000000000000	0.0000099729999970	0.4/81000210000050	Г	Г	Г Т
0.5000000000000000000000000000000000000	0.5450/50540522525	0.7110433000943040	т	т Т	I T
0.5000000000000000000000000000000000000	0.0341201199077433	0.7110433006943640	I E	I E	I E
0.5000000000000000000000000000000000000	0.555550001000002	0.3294300120000031	Г	Г	Г Б
0.5000000000000000000000000000000000000	0.000009972999970	0.3294300120000031	Г Б	Г Б	F E
0.5000000000000000000000000000000000000	0.0000000000000000000000000000000000000	0.4/81000210000050	Г	Г	Г
0.5000000000000000000000000000000000000	-0.000000000000000000000000000000000000	0.7007778334002032	I E	T E	
0.50000000000000000	0.0000000000000000000000000000000000000	0.5294300120000051	F	F	F E
0.8996900289999985	0.5000000000000000000000000000000000000	0.1999399970000013	F	F	
0.1003099989999967	0.50000000000000000	0.1999399970000013	Г	F	
0.1526200010000025	0.5000000000000000000000000000000000000	0.4038000130000015	F	F	F
0.84/3800089999983	0.50000000000000000	0.4038000130000015	F	F	F
0.34/38000899999983	0.50000000000000000	0.4038000130000015	F	F	F
0.6526199540000022	0.50000000000000000	0.4038000130000015	F	F	F
0.382/110650602688	0.50000000000000000	0.8059828387766678	I	I	I T
0.6172889349397311	0.50000000000000000	0.8059828387766678	T	T	T
0.09/920/0492/0410	0.5000000000000000000000000000000000000	0.5937734116759990	T	T	1
0.9020/93410729556	0.500000000000000000	0.5937734116759990	Т	T	T
0.1528865247295780	0.50000000000000000	0.7957939359747010	Т	T	T
0.8471134282704289	0.50000000000000000	0.7957939359747010	Т	T	T
0.3996899919999990	0.50000000000000000	0.1999399970000013	F	F	F
0.6003099710000015	0.500000000000000000	0.1999399970000013	F	F	F
0.5972112047469186	0.50000000000000000	0.5922958606449015	Т	Т	T
0.4027887952530814	0.50000000000000000	0.5922958606449015	Т	Т	Т
0.50000000000000000	0.50000000000000000	0.7600514605517775	Т	Т	Т

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