

Supplemental Material

Structure and Registry of the Silica Bilayer Film on Ru(0001) as Viewed by LEED and DFT

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1. Work function of Ru(0001)

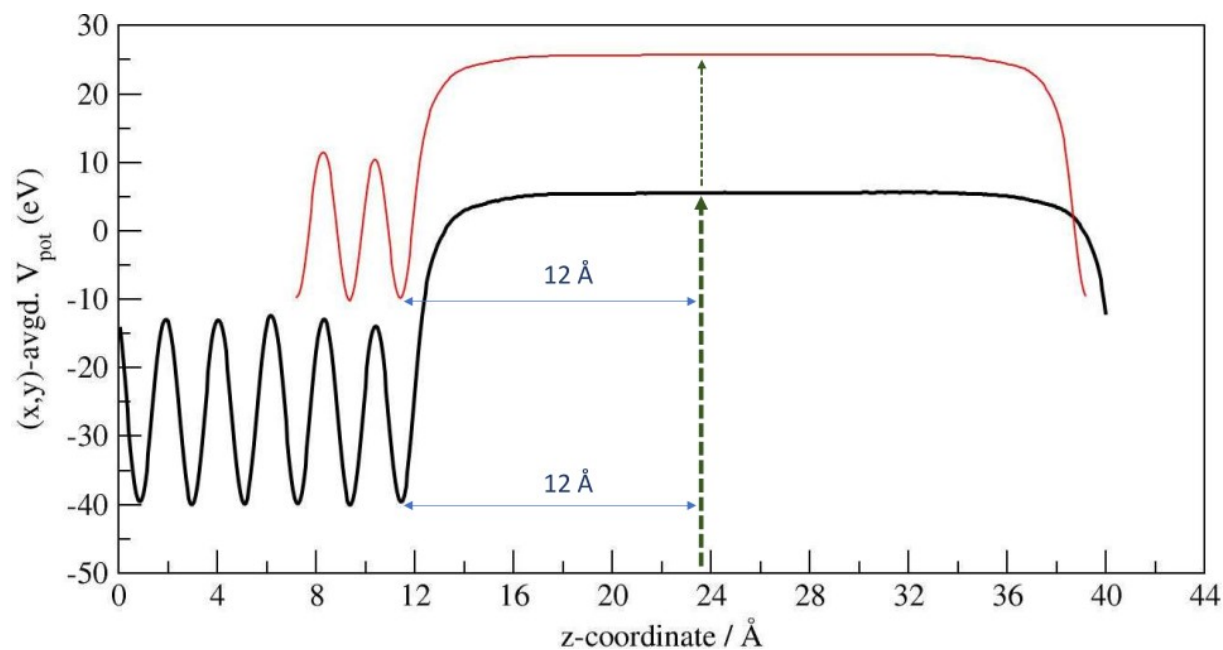


Figure S1. Work functions of slab models containing 6 (black line) and 3 (red line) Ru layers. The employed vacuum region of 12 Å is indicated by blue arrows. It is shown that the vacuum level of the surface is properly reached (zero slope) at this vacuum distance.

2. PES scans for the SiO₂ bi-layer in vertical direction to the substrate

Comparison of four dispersion-corrections for DFT (PBE-GGA):

1. Grimme's D2 approach [1-2]: Adapted to D2' – implies Krypton C₆ coefficients for Ru atoms (valence electrons are delocalized – Kr core remains – polarizability stems from Kr core electrons. Note that the first column in Tab. S1 shows PBE+D2 results obtained with default C₆ coefficients.
2. Grimme's D3 [3-4] approach with Becke-Johnson damping [5].
3. Steinmann's and Corminboeuf's dDsC (= density-dependent dispersion correction) [6-7].
4. Tkatchenko's and Scheffler's TS ansatz [8-9].

Table S1. Equilibrium distances (Å) at T = 0 K between film and substrate for optimized/minimum energy structures for different dispersion-corrections to the PBE functional. These distances have been obtained using a 6th order polynomial fit and refer to the vertical scans shown in Figs. S3-S5.

	PBE+D2 ^a	PBE+D2'	PBE+D3	PBE+dDsC	PBE+TS
Ru(0001)	2.68	2.87	2.69	3.27	2.72
1O-(2×2)	3.09	3.26	3.30	3.55	3.29
3O-(2×2)	3.81	3.90	3.89	3.97	3.78

^a Results obtained with default C₆ coefficients.

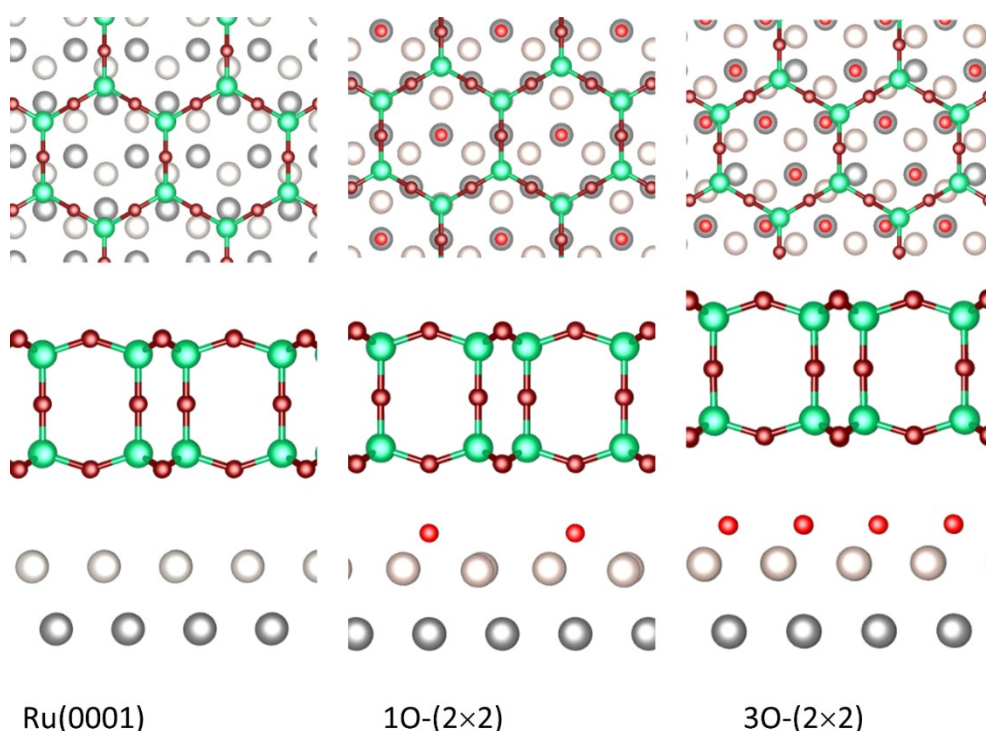


Figure S2. Top views (upper panel) and side views (lower panel) of the SiO₂ bi-layer on different substrates with increasing oxygen coverage. These structures correspond to (lateral) positions of the bi-layer relating to energy minima (see Figs. 4-6 in main text). Color code: Si is green, O atoms in bi-layer are dark red, interfacial O atoms on the surface are light red, Ru surface atoms are light gray, Ru subsurface atoms are dark grey.

2.1. SiO₂ on Ru(0001)

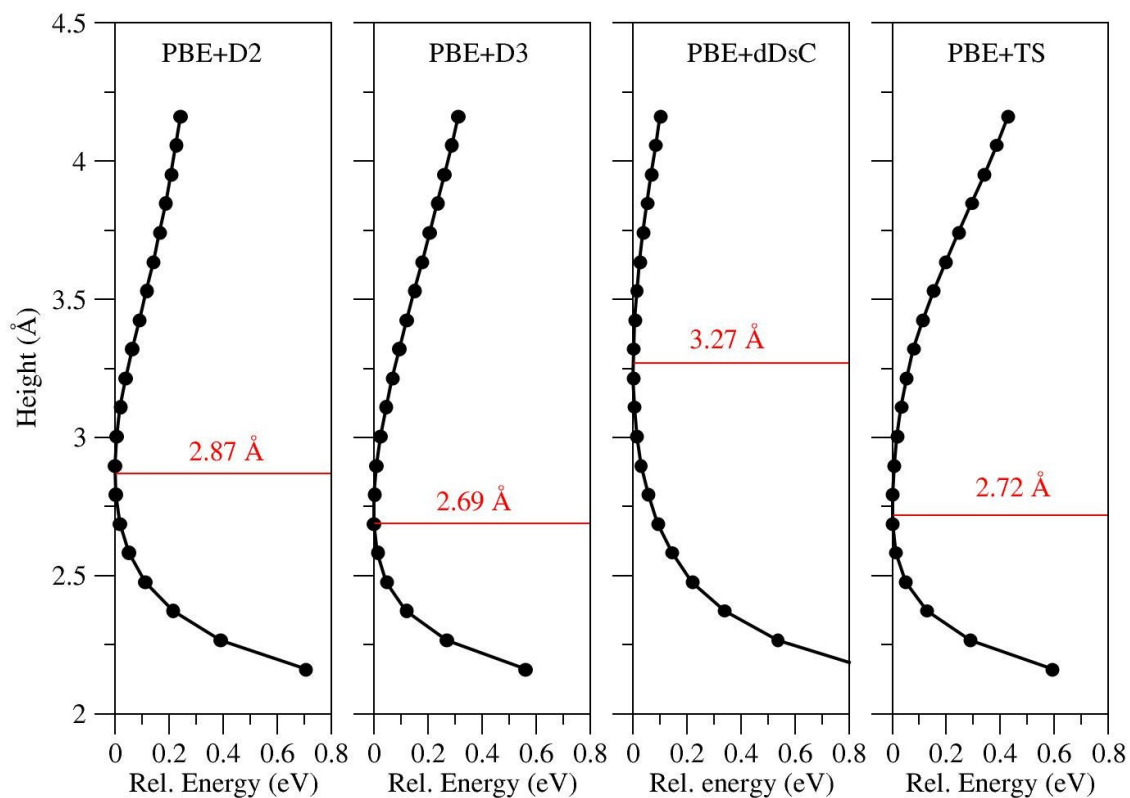


Figure S3. Cross section of the PES shifting the SiO₂ bi-layer vertically to the Ru(0001) substrate obtained using four different corrections to dispersion interaction as mentioned above (p. S4). The lateral position of the bi-layer corresponds to energy minima as shown in Fig. 4 (main text). Red lines mark heights (in Å) of minimal energy, which were obtained by virtue of a 6th order polynomial fit.

2.2. SiO₂ on 1O-(2×2)-Ru(0001)

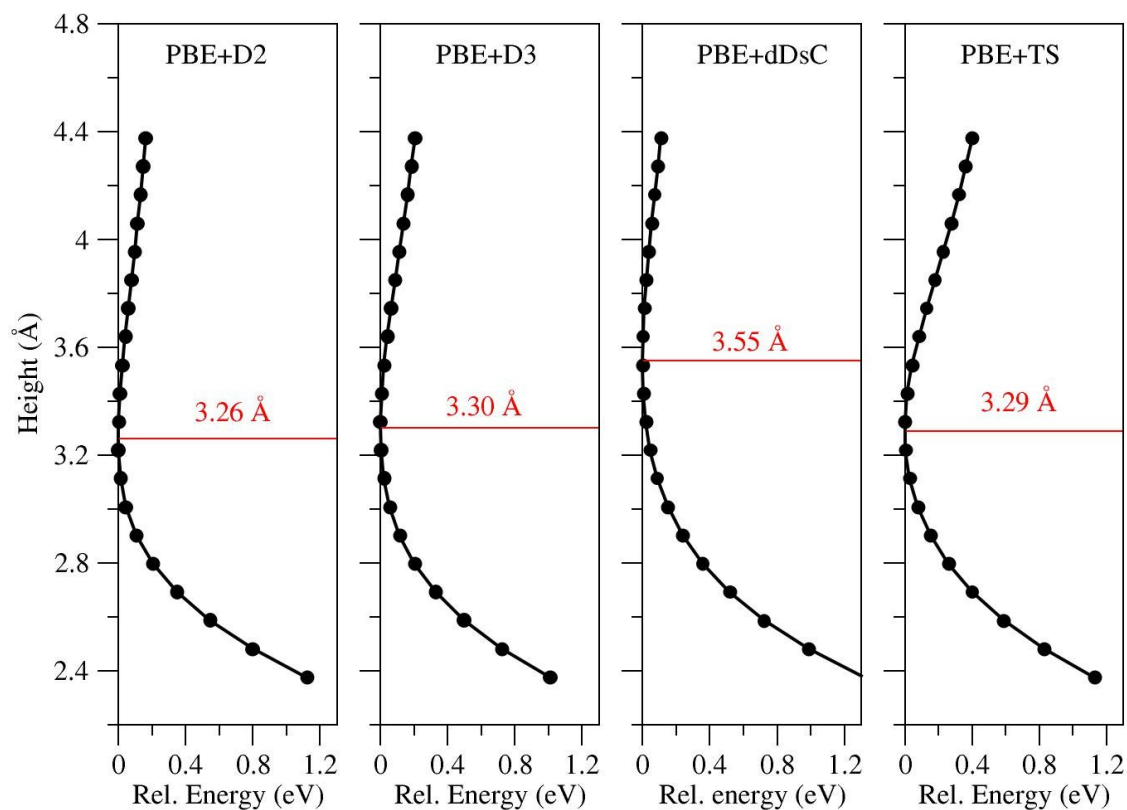


Figure S4. Cross section of the PES shifting the SiO₂ bi-layer vertically to the 1O-(2×2) Ru(0001) substrate obtained using four different corrections to dispersion interaction as mentioned above (p. S4). The lateral position of the bi-layer corresponds to energy minima as shown in Fig. 5 (main text). Red lines mark heights (in Å) of minimal energy, which were obtained by virtue of a 6th order polynomial fit.

2.3. SiO₂ on 3O-(2×2)-Ru(0001)

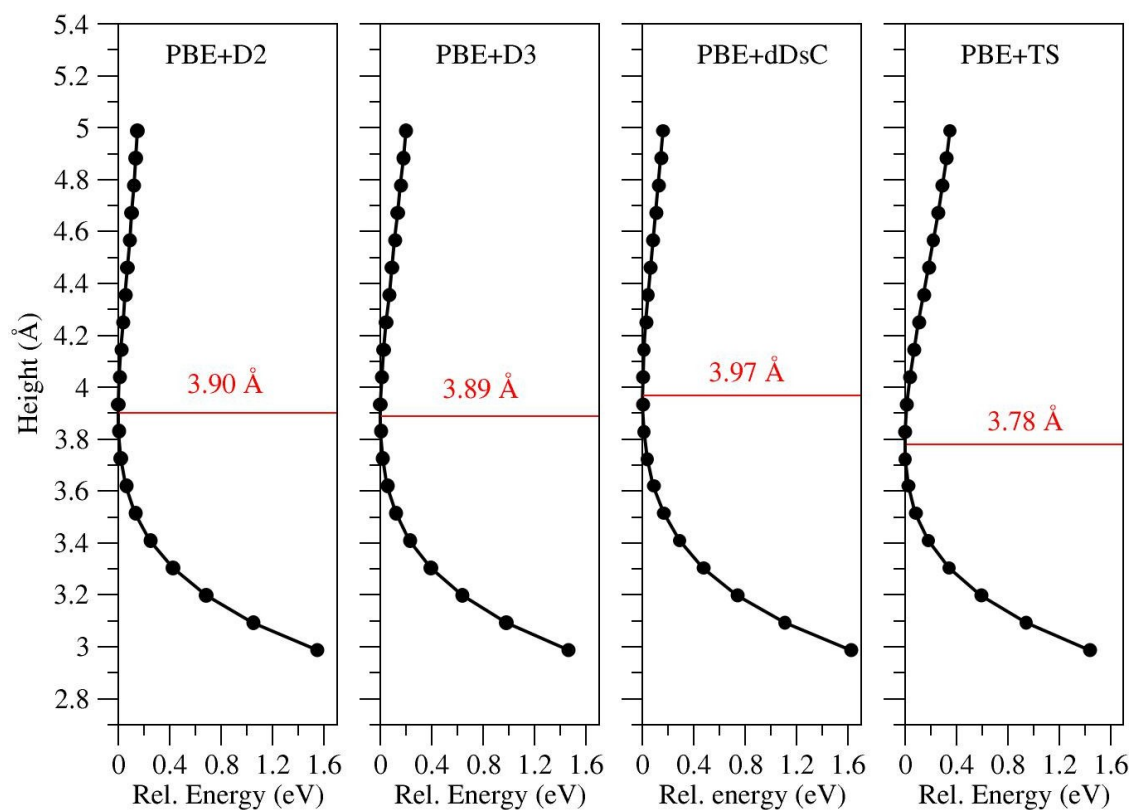


Figure S5. Cross section of the PES shifting the SiO₂ bi-layer vertically to the 3O-(2×2) Ru(0001) substrate obtained using four different corrections to dispersion interaction as mentioned above (p. S4). The lateral position of the bi-layer corresponds to energy minima as shown in Fig. 6 (main text). Red lines mark heights (in Å) of minimal energy, which were obtained by virtue of a 6th order polynomial fit.

3. van der Waals parameters employed within DFT+D2'

Table S2. C_6 parameters and van der Waals radii, R_0 , used in this work.

	$C_6 / \text{J}\cdot\text{nm}^6 \cdot \text{mol}^{-1}$	$R_0 / \text{\AA}$
Ru (= [Kr])	12.01	1.727
Si	9.23	1.716
O	0.70	1.342

4. Film-Substrate Orientations

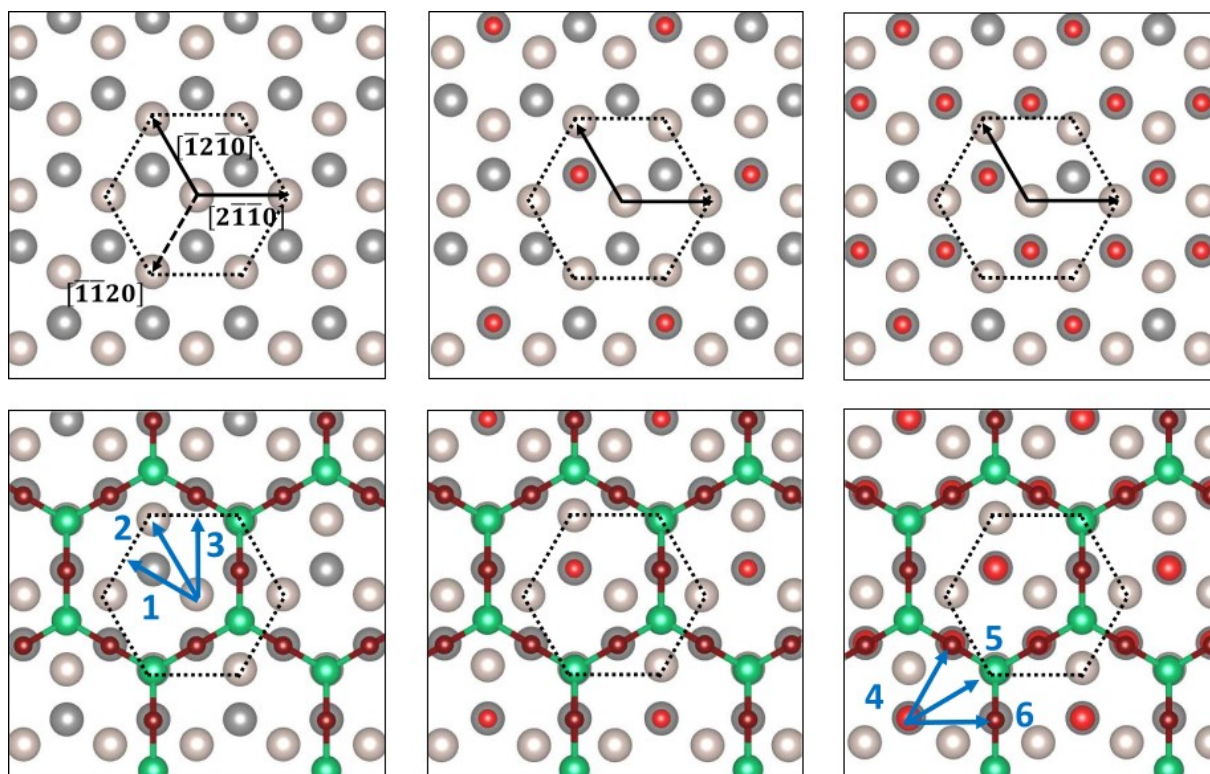


Figure S6. Top views on bare (left), 1O-(2×2) (middle), and 3O-(2×2) (right) Ru(0001) systems. The upper panel shows substrates, and the lower panel shows these systems covered by the silica bi-layer. Directions used in calculations of cross-sections through potential energy surfaces are displayed by blue arrows. Colour code: Surface Ru atoms are light grey, subsurface Ru is dark grey, surface O atoms are light red, Si atoms are green, and bilayer O atoms are dark red.

5. Cross Sections through PES of Ru(0001)

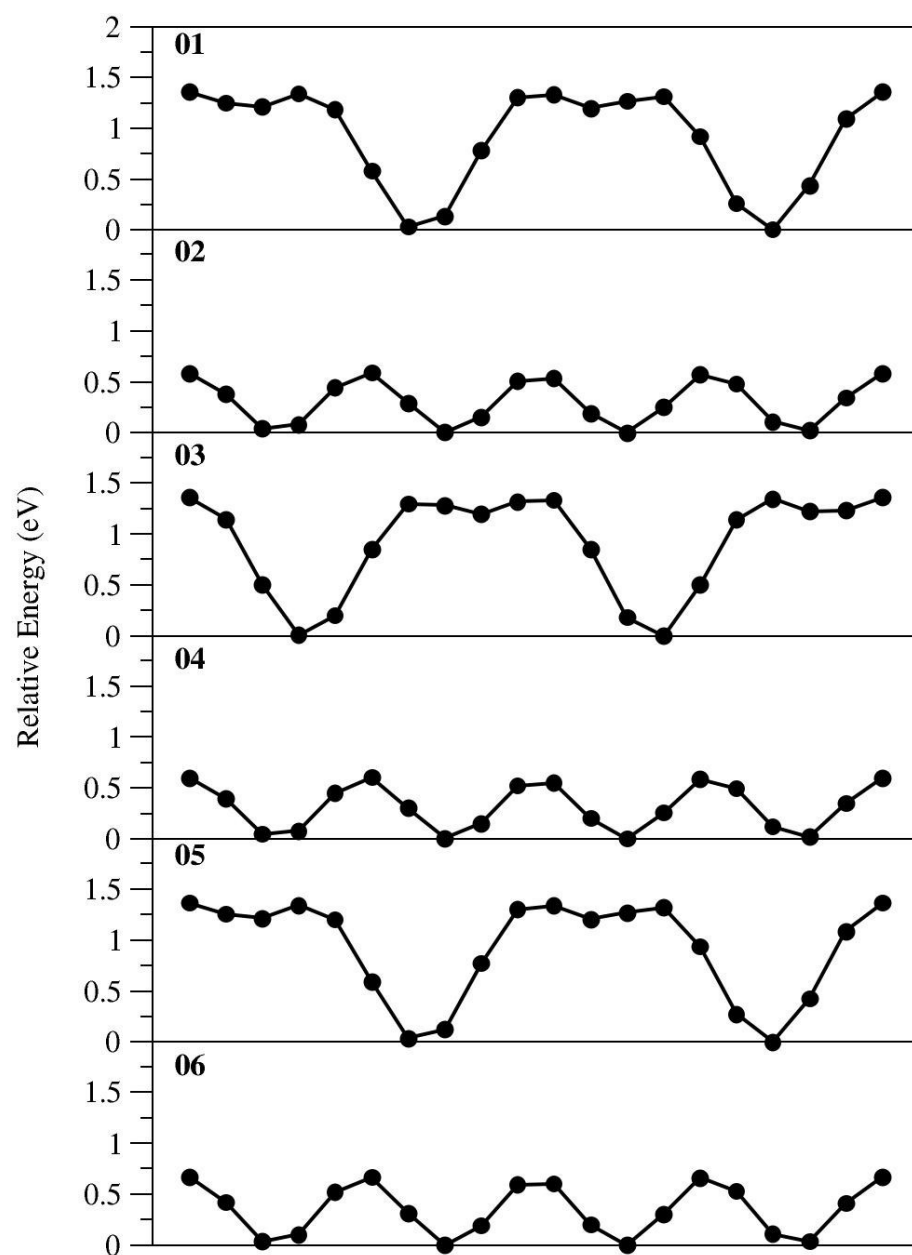


Figure S7. Cross sections through the potential energy surfaces obtained using PBE+D2' along six different crystallographic directions (see Fig. S6) for the silica bilayer on the bare Ru(0001) substrate.

6. Cross Sections through PES of 1O-(2×2) Ru(0001)

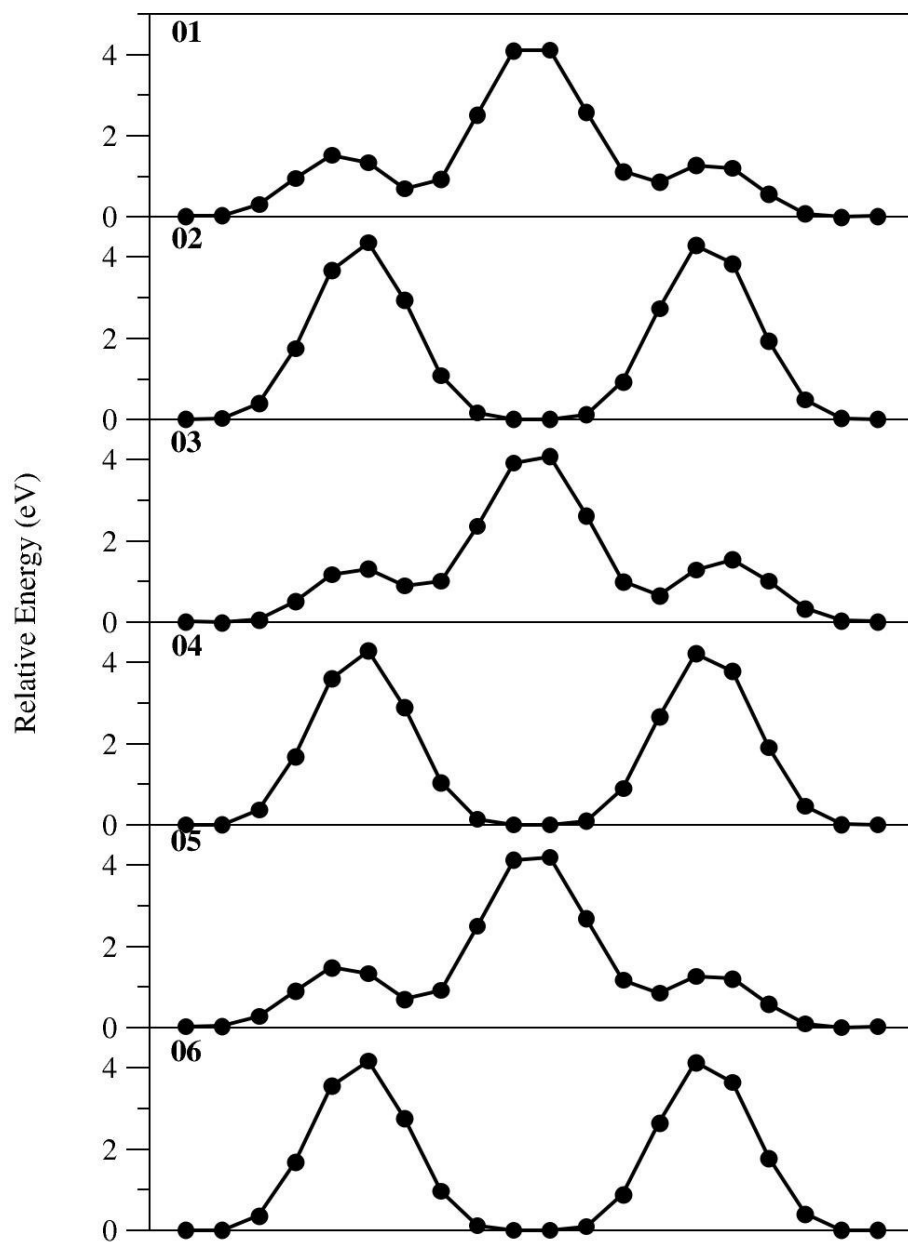


Figure S8. Cross sections through the potential energy surfaces obtained using PBE+D2' along six different crystallographic directions (see Fig. S6) for the silica bilayer on the 1O-(2×2) overlayer on Ru(0001).

7. Cross Sections through PES of 3O-(2×2) Ru(0001)

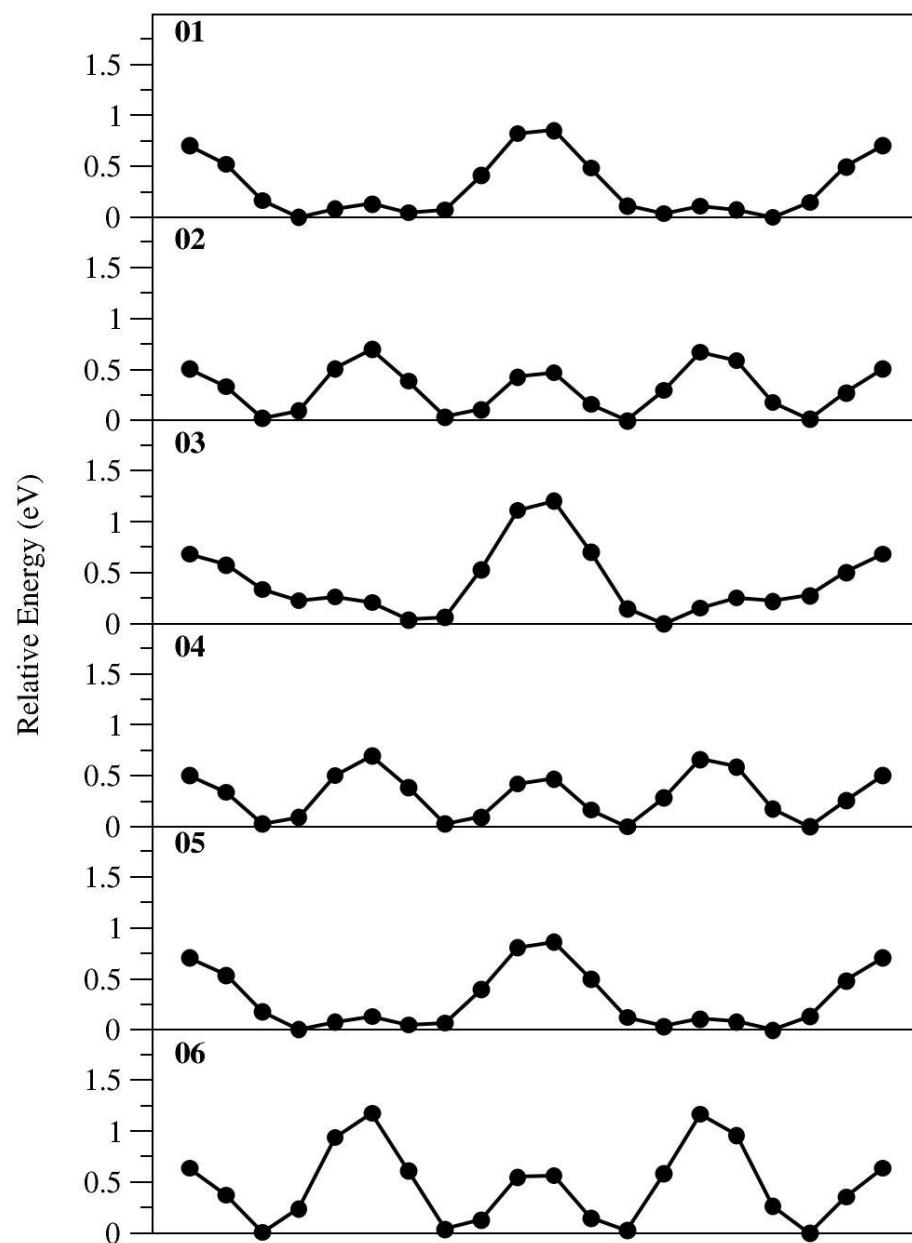


Figure S9. Cross sections through the potential energy surfaces obtained using PBE+D2' along six different crystallographic directions (see Fig. S6) for the silica bilayer on the 3O-(2×2) overlayer on Ru(0001).

8. x-, y-, and z-components of $[u]$ averaged over all O-atoms of the silica bilayer

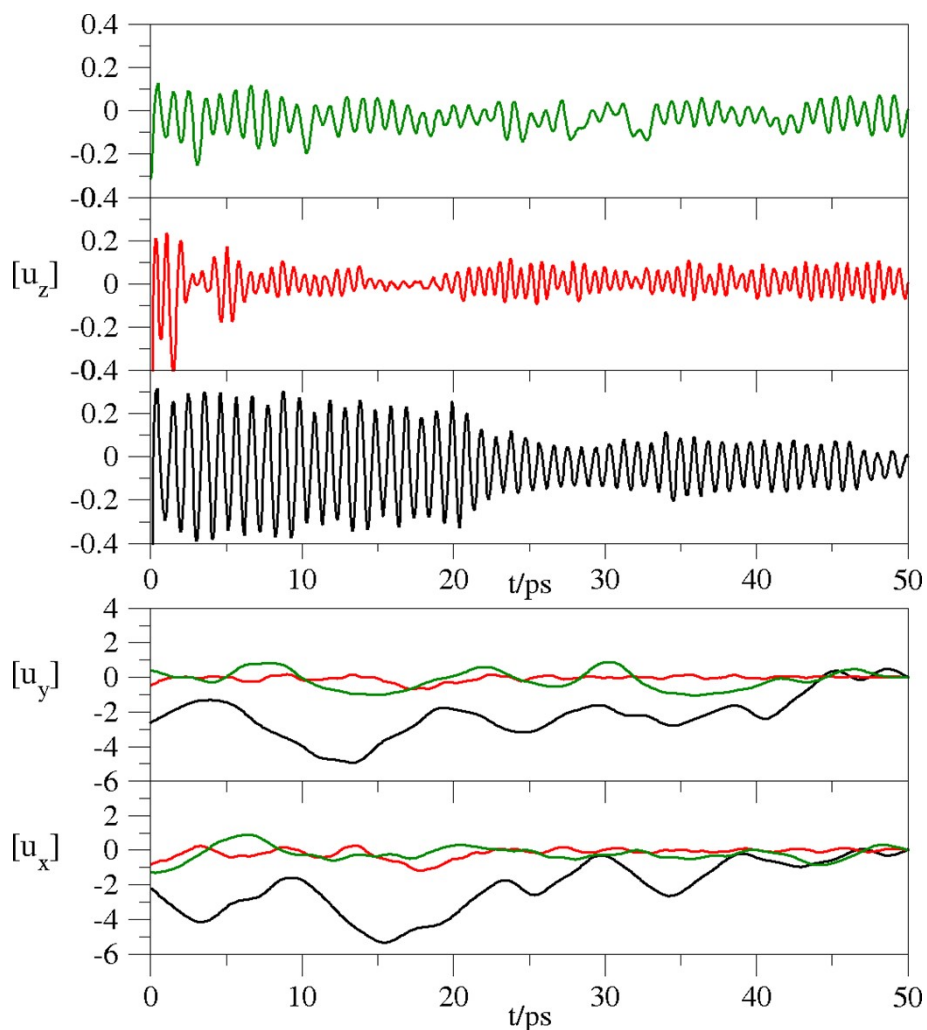


Figure S10. Deviations or amplitudes (Å) as a function of time t (ps) for the O atoms in the bilayer in x-, y, and z-directions with respect to the final structure obtained using MLFF-MD simulations. These time-evolutions are shown for the clean Ru(0001) (black), 1O (red), and 3O (green) systems. For clarity reasons, the upper three panels show amplitudes in z-direction for each system separately. Lower two panels show analogous results for coordinates parallel to the surfaces (i.e., x and y) collectively.

9. Models used for the LEED-I/V analysis

Table S2. List of all trial models considered in the LEED analysis with achieved R_p factors.

model class	model	R_p factors
high-symmetry adsorption site models	01) <i>fcc</i>	0.65
	02) <i>fcc</i> ₍₁₀₎	0.53
	03) <i>fcc</i> ₍₂₀₎	0.50
	04) <i>fcc</i> ₍₃₀₎	0.44
	05) <i>hcp</i>	0.69
	06) <i>hcp</i> ₍₁₀₎	0.62
	07) <i>hcp</i> ₍₂₀₎	0.57
	08) <i>hcp</i> ₍₃₀₎	0.51
	09) <i>top</i>	0.67
	10) <i>top</i> ₍₁₀₎	0.62
	11) <i>top</i> ₍₂₀₎	0.59
	12) <i>top</i> ₍₃₀₎	0.50
	13) (<i>fcc-hcp</i>)	0.71
	14) (<i>fcc-hcp</i>) ₍₁₀₎	0.66
	15) (<i>fcc-hcp</i>) ₍₂₀₎	0.63
	16) (<i>fcc-hcp</i>) ₍₃₀₎	0.47
mixed-O coverage	17) <i>fcc</i> ₍₁₀₊₂₀₎	0.48
	18) <i>fcc</i> ₍₁₀₊₃₀₎	0.42
	19) <i>fcc</i> ₍₂₀₊₃₀₎	0.49
	20) <i>fcc</i> ₍₁₀₊₂₀₊₃₀₎	0.41
	21) <i>hcp</i> ₍₁₀₊₂₀₎	0.55
	22) <i>hcp</i> ₍₁₀₊₃₀₎	0.48
	23) <i>hcp</i> ₍₂₀₊₃₀₎	0.50
	24) <i>hcp</i> ₍₁₀₊₂₀₊₃₀₎	0.50
	25) <i>top</i> ₍₁₀₊₂₀₎	0.57
	26) <i>top</i> ₍₁₀₊₃₀₎	0.49
	27) <i>top</i> ₍₂₀₊₃₀₎	0.48
	28) <i>top</i> ₍₁₀₊₂₀₊₃₀₎	0.49
	29) (<i>fcc-hcp</i>) ₍₁₀₊₂₀₎	0.60
	30) (<i>fcc-hcp</i>) ₍₁₀₊₃₀₎	0.45
	31) (<i>fcc-hcp</i>) ₍₂₀₊₃₀₎	0.46
	32) (<i>fcc-hcp</i>) ₍₁₀₊₂₀₊₃₀₎	0.43
split-position models (parallel to the surface)	33) <i>fcc</i> _(split)	0.29
	34) <i>hcp</i> _(split)	0.29
	35) <i>top</i> _(split)	0.32
	36) (<i>fcc-hcp</i>) _(split)	0.37

stacking disorder + split-position models	37) $fcc_{(split)} + hcp_{(split)}$	0.22
	38) $fcc_{(split)} + top_{(split)}$	0.23
	39) $fcc_{(split)} + (fcc-hcp)_{(split)}$	0.24
	40) $hcp_{(split)} + top_{(split)}$	0.25
	41) $hcp_{(split)} + (fcc-hcp)_{(split)}$	0.24
	42) $top_{(split)} + (fcc-hcp)_{(split)}$	0.27
	43) $fcc_{(split)} + hcp_{(split)} + top_{(split)}$	0.20
	44) $fcc_{(split)} + hcp_{(split)} + (fcc-hcp)_{(split)}$	0.21
	45) $fcc_{(split)} + top_{(split)} + (fcc-hcp)_{(split)}$	0.22
	46) $hcp_{(split)} + top_{(split)} + (fcc-hcp)_{(split)}$	0.23
	47) $fcc_{(split)} + hcp_{(split)} + top_{(split)} + (fcc-hcp)_{(split)}$	0.16

Table S3. List of experimental LEED spots used for the analysis with achieved R_p factors for model 47.

Spot	ΔE range	R_p
(0,1/2)	49.00 to 137.00 eV	0.25
(1/2,1/2)	45.00 to 300.00 eV	0.29
(0,1)	50.00 to 500.00 eV	0.10
(1/2,1)	110.00 to 300.00 eV	0.18
(1,1)	180.00 to 500.00 eV	0.08
(0,3/2)	115.00 to 500.00 eV	0.22
(1/2,3/2)	170.00 to 480.00 eV	0.13
(0,2)	208.00 to 450.00 eV	0.14
(1/2,2)	290.00 to 480.00 eV	0.16
(1,3/2)	330.00 to 500.00 eV	0.08

The energy range is not the same for all beams, because the diffracted spots appear on the screen at different energies. Higher order spots (higher Miller indexes) appear at higher energies. The reason for that is the radius of the Ewald sphere in the reciprocal space increases as the energy of the incident beam increases. The intensities for (0,1/2) and (1/2,1/2) at energies above 137.00 eV and 300.00 eV, respectively were too weak to be measured. The same happens for the (1/2,3/2), (0,2) and (1/2,2) beams.

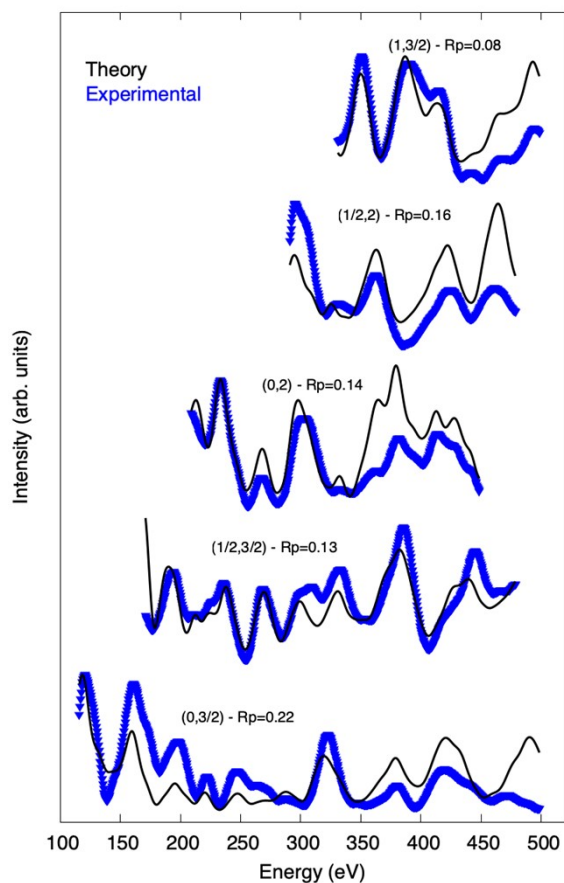


Figure S11. Analysis of further LEED spots. Experimental (blue) and theoretical (black) LEED-I/V curves for the best model($R_p=0.16$) obtained from the LEED analysis. The (i, j) notation gives the index of the diffraction spots. The R_p for each individual beam is also shown.

10. References

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11. Selected structure coordinates for the lateral or translational scans of the silica BL on Ru(0001), 1O, and 3O in the VASP POSCAR format

11.1. The Ru(0001) Substrate

Comment: Fig. 4 – first point (0.67 eV)

1.0

+16.2998100000 +0.0000000000 +0.0000000000
-8.1499200000 +14.1160500000 +0.0000000000
+0.0000000000 +0.0000000000 +24.0000000000

Ru Si O

108 36 72

Selective

Cartesian

+1.3583000000 +2.3527000000 +1.0000000000 F F F
-1.3583000000 +2.3527000000 +1.0000000000 F F F
+2.7166000000 +0.0000000000 +1.0000000000 F F F
+0.0000000000 +0.0000000000 +1.0000000000 F F F
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 -4.0824206935 +13.2956318432 +12.1374828913 T T T
 -1.3658024845 +11.7267132968 +12.1396056153 T T T
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 +6.7853182174 +3.8841951840 +8.8882526853 T T T
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 -0.0065227700 +3.0991489813 +8.3780081729 T T T
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 +1.3523442905 +5.4527917913 +8.3764901632 T T T
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 -2.7242664656 +12.5114061361 +12.6532764187 T T T
 -1.3660224191 +10.1582506360 +12.6544034288 T T T
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 -1.3642957095 +10.1581417913 +8.3764901632 T T T
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 +8.1422835344 +3.1007061361 +12.6532764187 T T T
 +9.5005275809 +0.7475506360 +12.6544034288 T T T
 +6.7847475878 +3.8858245868 +10.5122953107 T T T
 +9.5011195823 +2.3145980137 +10.5145987526 T T T
 +9.5022542905 +0.7474417913 +8.3764901632 T T T
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 +4.0672475809 +10.1582506360 +12.6544034288 T T T
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 +8.1439870460 +12.5101850744 +8.3778210771 T T T
 +5.4267372300 +12.5098489813 +8.3780081729 T T T

commentline Fig. 4 - 8th point (0.0 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

0.000000000 0.000000000 24.000000000

Ru Si O

108 36 72

Selective

Cartesian

1.358300000000	2.352700000000	1.000000000000	F	F	F
-1.358300000000	2.352700000000	1.000000000000	F	F	F
2.716600000000	0.000000000000	1.000000000000	F	F	F
0.000000000000	0.000000000000	1.000000000000	F	F	F
1.358300000000	0.784200000000	3.141100000000	F	F	F
4.075000000000	0.784200000000	3.141100000000	F	F	F
0.000000000000	3.136900000000	3.141100000000	F	F	F
2.716600000000	3.136900000000	3.141100000000	F	F	F
1.358312238800	2.352741666300	5.193448999800	T	T	T
4.075112645700	2.353521319700	5.184454391300	T	T	T
0.000204066800	4.705661034200	5.193491229800	T	T	T
2.716589994700	4.705639284500	5.193549923200	T	T	T
-1.358340000000	7.058050000000	1.000000000000	F	F	F
-4.074940000000	7.058050000000	1.000000000000	F	F	F
-0.000040000000	4.705350000000	1.000000000000	F	F	F
-2.716640000000	4.705350000000	1.000000000000	F	F	F
-1.358340000000	5.489550000000	3.141100000000	F	F	F
1.358360000000	5.489550000000	3.141100000000	F	F	F
-2.716640000000	7.842250000000	3.141100000000	F	F	F
-0.000040000000	7.842250000000	3.141100000000	F	F	F
-1.358327761200	7.058091666300	5.193448999800	T	T	T
1.358472645700	7.058871319700	5.184454391300	T	T	T
-2.716435933200	9.411011034200	5.193491229800	T	T	T
-0.000050005300	9.410989284500	5.193549923200	T	T	T
-4.074980000000	11.763400000000	1.000000000000	F	F	F
-6.791580000000	11.763400000000	1.000000000000	F	F	F
-2.716680000000	9.410700000000	1.000000000000	F	F	F
-5.433280000000	9.410700000000	1.000000000000	F	F	F
-4.074980000000	10.194900000000	3.141100000000	F	F	F
-1.358280000000	10.194900000000	3.141100000000	F	F	F
-5.433280000000	12.547600000000	3.141100000000	F	F	F
-2.716680000000	12.547600000000	3.141100000000	F	F	F
-4.074967761200	11.763441666300	5.193448999800	T	T	T
-1.358167354300	11.764221319700	5.184454391300	T	T	T
-5.433075933200	14.116361034200	5.193491229800	T	T	T
-2.716690005300	14.116339284500	5.193549923200	T	T	T
6.791570000000	2.352700000000	1.000000000000	F	F	F
4.074970000000	2.352700000000	1.000000000000	F	F	F
8.149870000000	0.000000000000	1.000000000000	F	F	F
5.433270000000	0.000000000000	1.000000000000	F	F	F
6.791570000000	0.784200000000	3.141100000000	F	F	F
9.508270000000	0.784200000000	3.141100000000	F	F	F
5.433270000000	3.136900000000	3.141100000000	F	F	F
8.149870000000	3.136900000000	3.141100000000	F	F	F
6.791582238800	2.352741666300	5.193448999800	T	T	T

9.508382645700	2.353521319700	5.184454391300	T T T
5.433474066800	4.705661034200	5.193491229800	T T T
8.149859994700	4.705639284500	5.193549923200	T T T
4.074930000000	7.058050000000	1.000000000000	F F F
1.358330000000	7.058050000000	1.000000000000	F F F
5.433230000000	4.705350000000	1.000000000000	F F F
2.716630000000	4.705350000000	1.000000000000	F F F
4.074930000000	5.489550000000	3.141100000000	F F F
6.791630000000	5.489550000000	3.141100000000	F F F
2.716630000000	7.842250000000	3.141100000000	F F F
5.433230000000	7.842250000000	3.141100000000	F F F
4.074942238800	7.058091666300	5.193448999800	T T T
6.791742645700	7.058871319700	5.184454391300	T T T
2.716834066800	9.411011034200	5.193491229800	T T T
5.433219994700	9.410989284500	5.193549923200	T T T
1.358290000000	11.763400000000	1.000000000000	F F F
-1.358310000000	11.763400000000	1.000000000000	F F F
2.716590000000	9.410700000000	1.000000000000	F F F
-0.000010000000	9.410700000000	1.000000000000	F F F
1.358290000000	10.194900000000	3.141100000000	F F F
4.074990000000	10.194900000000	3.141100000000	F F F
-0.000010000000	12.547600000000	3.141100000000	F F F
2.716590000000	12.547600000000	3.141100000000	F F F
1.358302238800	11.763441666300	5.193448999800	T T T
4.075102645700	11.764221319700	5.184454391300	T T T
0.000194066800	14.116361034200	5.193491229800	T T T
2.716579994700	14.116339284500	5.193549923200	T T T
12.224840000000	2.352700000000	1.000000000000	F F F
9.508240000000	2.352700000000	1.000000000000	F F F
13.583140000000	0.000000000000	1.000000000000	F F F
10.866540000000	0.000000000000	1.000000000000	F F F
12.224840000000	0.784200000000	3.141100000000	F F F
14.941540000000	0.784200000000	3.141100000000	F F F
10.866540000000	3.136900000000	3.141100000000	F F F
13.583140000000	3.136900000000	3.141100000000	F F F
12.224852238800	2.352741666300	5.193448999800	T T T
14.941652645700	2.353521319700	5.184454391300	T T T
10.866744066800	4.705661034200	5.193491229800	T T T
13.583129994700	4.705639284500	5.193549923200	T T T
9.508200000000	7.058050000000	1.000000000000	F F F
6.791600000000	7.058050000000	1.000000000000	F F F
10.866500000000	4.705350000000	1.000000000000	F F F
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9.508200000000	5.489550000000	3.141100000000	F F F
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8.149900000000	7.842250000000	3.141100000000	F F F
10.866500000000	7.842250000000	3.141100000000	F F F
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5.433260000000	9.410700000000	1.000000000000	F F F
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5.433260000000	12.547600000000	3.141100000000	F F F

8.149860000000	12.547600000000	3.141100000000	F F F
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5.354321360629	3.884931843200	12.137482891300	T T T
8.070939569629	2.316013296800	12.139605615300	T T T
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8.072096983329	2.315242773000	8.892393552400	T T T
2.637681360629	8.590281843200	12.137482891300	T T T
5.354299569629	7.021363296800	12.139605615300	T T T
2.638870271529	8.589545184000	8.888252685300	T T T
5.355456983329	7.020592773000	8.892393552400	T T T
-0.078958639371	13.295631843200	12.137482891300	T T T
2.637659569629	11.726713296800	12.139605615300	T T T
-0.077769728471	13.294895184000	8.888252685300	T T T
2.638816983329	11.725942773000	8.892393552400	T T T
10.787591360629	3.884931843200	12.137482891300	T T T
13.504209569629	2.316013296800	12.139605615300	T T T
10.788780271529	3.884195184000	8.888252685300	T T T
13.505366983329	2.315242773000	8.892393552400	T T T
8.070951360629	8.590281843200	12.137482891300	T T T
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8.072140271529	8.589545184000	8.888252685300	T T T
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18.937479569629	2.316013296800	12.139605615300	T T T
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16.221996983329	7.020592773000	8.892393552400	T T T
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13.505356983329	11.725942773000	8.892393552400	T T T
3.996113364529	3.100839093400	12.653156449400	T T T
6.712475588529	3.100706136100	12.653276418700	T T T
8.070719635029	0.747550636000	12.654403428800	T T T
5.354939641929	3.885824586800	10.512295310700	T T T
8.071311636429	2.314598013700	10.514598752600	T T T
8.072446344629	0.747441791300	8.376490163200	T T T
6.714189100129	3.099485074400	8.377821077100	T T T
3.996939284129	3.099148981300	8.378008172900	T T T
1.279473364529	7.806189093400	12.653156449400	T T T
3.995835588529	7.806056136100	12.653276418700	T T T
5.354079635029	5.452900636000	12.654403428800	T T T
2.638299641929	8.591174586800	10.512295310700	T T T
5.354671636429	7.019948013700	10.514598752600	T T T
5.355806344629	5.452791791300	8.376490163200	T T T
3.997549100129	7.804835074400	8.377821077100	T T T
1.280299284129	7.804498981300	8.378008172900	T T T
-1.437166635471	12.511539093400	12.653156449400	T T T

1.279195588529	12.511406136100	12.653276418700	T T T
2.637439635029	10.158250636000	12.654403428800	T T T
-0.078340358071	13.296524586800	10.512295310700	T T T
2.638031636429	11.725298013700	10.514598752600	T T T
2.639166344629	10.158141791300	8.376490163200	T T T
1.280909100129	12.510185074400	8.377821077100	T T T
-1.436340715871	12.509848981300	8.378008172900	T T T
9.429383364529	3.100839093400	12.653156449400	T T T
12.145745588529	3.100706136100	12.653276418700	T T T
13.503989635029	0.747550636000	12.654403428800	T T T
10.788209641929	3.885824586800	10.512295310700	T T T
13.504581636429	2.314598013700	10.514598752600	T T T
13.505716344629	0.747441791300	8.376490163200	T T T
12.147459100129	3.099485074400	8.377821077100	T T T
9.430209284129	3.099148981300	8.378008172900	T T T
6.712743364529	7.806189093400	12.653156449400	T T T
9.429105588529	7.806056136100	12.653276418700	T T T
10.787349635029	5.452900636000	12.654403428800	T T T
8.071569641929	8.591174586800	10.512295310700	T T T
10.787941636429	7.019948013700	10.514598752600	T T T
10.789076344629	5.452791791300	8.376490163200	T T T
9.430819100129	7.804835074400	8.377821077100	T T T
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3.996103364529	12.511539093400	12.653156449400	T T T
6.712465588529	12.511406136100	12.653276418700	T T T
8.070709635029	10.158250636000	12.654403428800	T T T
5.354929641929	13.296524586800	10.512295310700	T T T
8.071301636429	11.725298013700	10.514598752600	T T T
8.072436344629	10.158141791300	8.376490163200	T T T
6.714179100129	12.510185074400	8.377821077100	T T T
3.996929284129	12.509848981300	8.378008172900	T T T
14.862653364529	3.100839093400	12.653156449400	T T T
17.579015588529	3.100706136100	12.653276418700	T T T
18.937259635029	0.747550636000	12.654403428800	T T T
16.221479641929	3.885824586800	10.512295310700	T T T
18.937851636429	2.314598013700	10.514598752600	T T T
18.938986344629	0.747441791300	8.376490163200	T T T
17.580729100129	3.099485074400	8.377821077100	T T T
14.863479284129	3.099148981300	8.378008172900	T T T
12.146013364529	7.806189093400	12.653156449400	T T T
14.862375588529	7.806056136100	12.653276418700	T T T
16.220619635029	5.452900636000	12.654403428800	T T T
13.504839641929	8.591174586800	10.512295310700	T T T
16.221211636429	7.019948013700	10.514598752600	T T T
16.222346344629	5.452791791300	8.376490163200	T T T
14.864089100129	7.804835074400	8.377821077100	T T T
12.146839284129	7.804498981300	8.378008172900	T T T
9.429373364529	12.511539093400	12.653156449400	T T T
12.145735588529	12.511406136100	12.653276418700	T T T
13.503979635029	10.158250636000	12.654403428800	T T T
10.788199641929	13.296524586800	10.512295310700	T T T
13.504571636429	11.725298013700	10.514598752600	T T T
13.505706344629	10.158141791300	8.376490163200	T T T
12.147449100129	12.510185074400	8.377821077100	T T T
9.430199284129	12.509848981300	8.378008172900	T T T

commentline Fig. 4 – 11th point (0.60 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

0.000000000 0.000000000 24.000000000

Ru Si O

108 36 72

Selective

Cartesian

1.358300000000	2.352700000000	1.000000000000	F	F	F
-1.358300000000	2.352700000000	1.000000000000	F	F	F
2.716600000000	0.000000000000	1.000000000000	F	F	F
0.000000000000	0.000000000000	1.000000000000	F	F	F
1.358300000000	0.784200000000	3.141100000000	F	F	F
4.075000000000	0.784200000000	3.141100000000	F	F	F
0.000000000000	3.136900000000	3.141100000000	F	F	F
2.716600000000	3.136900000000	3.141100000000	F	F	F
1.358312238800	2.352741666300	5.193448999800	T	T	T
4.075112645700	2.353521319700	5.184454391300	T	T	T
0.000204066800	4.705661034200	5.193491229800	T	T	T
2.716589994700	4.705639284500	5.193549923200	T	T	T
-1.358340000000	7.058050000000	1.000000000000	F	F	F
-4.074940000000	7.058050000000	1.000000000000	F	F	F
-0.000040000000	4.705350000000	1.000000000000	F	F	F
-2.716640000000	4.705350000000	1.000000000000	F	F	F
-1.358340000000	5.489550000000	3.141100000000	F	F	F
1.358360000000	5.489550000000	3.141100000000	F	F	F
-2.716640000000	7.842250000000	3.141100000000	F	F	F
-0.000040000000	7.842250000000	3.141100000000	F	F	F
-1.358327761200	7.058091666300	5.193448999800	T	T	T
1.358472645700	7.058871319700	5.184454391300	T	T	T
-2.716435933200	9.411011034200	5.193491229800	T	T	T
-0.000050005300	9.410989284500	5.193549923200	T	T	T
-4.074980000000	11.763400000000	1.000000000000	F	F	F
-6.791580000000	11.763400000000	1.000000000000	F	F	F
-2.716680000000	9.410700000000	1.000000000000	F	F	F
-5.433280000000	9.410700000000	1.000000000000	F	F	F
-4.074980000000	10.194900000000	3.141100000000	F	F	F
-1.358280000000	10.194900000000	3.141100000000	F	F	F
-5.433280000000	12.547600000000	3.141100000000	F	F	F
-2.716680000000	12.547600000000	3.141100000000	F	F	F
-4.074967761200	11.763441666300	5.193448999800	T	T	T
-1.358167354300	11.764221319700	5.184454391300	T	T	T
-5.433075933200	14.116361034200	5.193491229800	T	T	T
-2.716690005300	14.116339284500	5.193549923200	T	T	T
6.791570000000	2.352700000000	1.000000000000	F	F	F
4.074970000000	2.352700000000	1.000000000000	F	F	F
8.149870000000	0.000000000000	1.000000000000	F	F	F
5.433270000000	0.000000000000	1.000000000000	F	F	F
6.791570000000	0.784200000000	3.141100000000	F	F	F
9.508270000000	0.784200000000	3.141100000000	F	F	F
5.433270000000	3.136900000000	3.141100000000	F	F	F
8.149870000000	3.136900000000	3.141100000000	F	F	F
6.791582238800	2.352741666300	5.193448999800	T	T	T
9.508382645700	2.353521319700	5.184454391300	T	T	T
5.433474066800	4.705661034200	5.193491229800	T	T	T

8.149859994700	4.705639284500	5.193549923200	T T T
4.074930000000	7.058050000000	1.000000000000	F F F
1.358330000000	7.058050000000	1.000000000000	F F F
5.433230000000	4.705350000000	1.000000000000	F F F
2.716630000000	4.705350000000	1.000000000000	F F F
4.074930000000	5.489550000000	3.141100000000	F F F
6.791630000000	5.489550000000	3.141100000000	F F F
2.716630000000	7.842250000000	3.141100000000	F F F
5.433230000000	7.842250000000	3.141100000000	F F F
4.074942238800	7.058091666300	5.193448999800	T T T
6.791742645700	7.058871319700	5.184454391300	T T T
2.716834066800	9.411011034200	5.193491229800	T T T
5.433219994700	9.410989284500	5.193549923200	T T T
1.358290000000	11.763400000000	1.000000000000	F F F
-1.358310000000	11.763400000000	1.000000000000	F F F
2.716590000000	9.410700000000	1.000000000000	F F F
-0.000010000000	9.410700000000	1.000000000000	F F F
1.358290000000	10.194900000000	3.141100000000	F F F
4.074990000000	10.194900000000	3.141100000000	F F F
-0.000010000000	12.547600000000	3.141100000000	F F F
2.716590000000	12.547600000000	3.141100000000	F F F
1.358302238800	11.763441666300	5.193448999800	T T T
4.075102645700	11.764221319700	5.184454391300	T T T
0.000194066800	14.116361034200	5.193491229800	T T T
2.716579994700	14.116339284500	5.193549923200	T T T
12.224840000000	2.352700000000	1.000000000000	F F F
9.508240000000	2.352700000000	1.000000000000	F F F
13.583140000000	0.000000000000	1.000000000000	F F F
10.866540000000	0.000000000000	1.000000000000	F F F
12.224840000000	0.784200000000	3.141100000000	F F F
14.941540000000	0.784200000000	3.141100000000	F F F
10.866540000000	3.136900000000	3.141100000000	F F F
13.583140000000	3.136900000000	3.141100000000	F F F
12.224852238800	2.352741666300	5.193448999800	T T T
14.941652645700	2.353521319700	5.184454391300	T T T
10.866744066800	4.705661034200	5.193491229800	T T T
13.583129994700	4.705639284500	5.193549923200	T T T
9.508200000000	7.058050000000	1.000000000000	F F F
6.791600000000	7.058050000000	1.000000000000	F F F
10.866500000000	4.705350000000	1.000000000000	F F F
8.149900000000	4.705350000000	1.000000000000	F F F
9.508200000000	5.489550000000	3.141100000000	F F F
12.224900000000	5.489550000000	3.141100000000	F F F
8.149900000000	7.842250000000	3.141100000000	F F F
10.866500000000	7.842250000000	3.141100000000	F F F
9.508212238800	7.058091666300	5.193448999800	T T T
12.225012645700	7.058871319700	5.184454391300	T T T
8.150104066800	9.411011034200	5.193491229800	T T T
10.866489994700	9.410989284500	5.193549923200	T T T
6.791560000000	11.763400000000	1.000000000000	F F F
4.074960000000	11.763400000000	1.000000000000	F F F
8.149860000000	9.410700000000	1.000000000000	F F F
5.433260000000	9.410700000000	1.000000000000	F F F
6.791560000000	10.194900000000	3.141100000000	F F F
9.508260000000	10.194900000000	3.141100000000	F F F
5.433260000000	12.547600000000	3.141100000000	F F F
8.149860000000	12.547600000000	3.141100000000	F F F
6.791572238800	11.763441666300	5.193448999800	T T T

9.508372645700	11.764221319700	5.184454391300	T T T
5.433464066800	14.116361034200	5.193491229800	T T T
8.149849994700	14.116339284500	5.193549923200	T T T
7.070091089983	3.884931843200	12.137482891300	T T T
9.786709298983	2.316013296800	12.139605615300	T T T
7.071280000883	3.884195184000	8.888252685300	T T T
9.787866712683	2.315242773000	8.892393552400	T T T
4.353451089983	8.590281843200	12.137482891300	T T T
7.070069298983	7.021363296800	12.139605615300	T T T
4.354640000883	8.589545184000	8.888252685300	T T T
7.071226712683	7.020592773000	8.892393552400	T T T
1.636811089983	13.295631843200	12.137482891300	T T T
4.353429298983	11.726713296800	12.139605615300	T T T
1.638000000883	13.294895184000	8.888252685300	T T T
4.354586712683	11.725942773000	8.892393552400	T T T
12.503361089983	3.884931843200	12.137482891300	T T T
15.219979298983	2.316013296800	12.139605615300	T T T
12.504550000883	3.884195184000	8.888252685300	T T T
15.221136712683	2.315242773000	8.892393552400	T T T
9.786721089983	8.590281843200	12.137482891300	T T T
12.503339298983	7.021363296800	12.139605615300	T T T
9.787910000883	8.589545184000	8.888252685300	T T T
12.504496712683	7.020592773000	8.892393552400	T T T
7.070081089983	13.295631843200	12.137482891300	T T T
9.786699298983	11.726713296800	12.139605615300	T T T
7.071270000883	13.294895184000	8.888252685300	T T T
9.787856712683	11.725942773000	8.892393552400	T T T
17.936631089983	3.884931843200	12.137482891300	T T T
20.653249298983	2.316013296800	12.139605615300	T T T
17.937820000883	3.884195184000	8.888252685300	T T T
20.654406712683	2.315242773000	8.892393552400	T T T
15.219991089983	8.590281843200	12.137482891300	T T T
17.936609298983	7.021363296800	12.139605615300	T T T
15.221180000883	8.589545184000	8.888252685300	T T T
17.937766712683	7.020592773000	8.892393552400	T T T
12.503351089983	13.295631843200	12.137482891300	T T T
15.219969298983	11.726713296800	12.139605615300	T T T
12.504540000883	13.294895184000	8.888252685300	T T T
15.221126712683	11.725942773000	8.892393552400	T T T
5.711883093883	3.100839093400	12.653156449400	T T T
8.428245317883	3.100706136100	12.653276418700	T T T
9.786489364383	0.747550636000	12.654403428800	T T T
7.070709371283	3.885824586800	10.512295310700	T T T
9.787081365783	2.314598013700	10.514598752600	T T T
9.788216073983	0.747441791300	8.376490163200	T T T
8.429958829483	3.099485074400	8.377821077100	T T T
5.712709013483	3.099148981300	8.378008172900	T T T
2.995243093883	7.806189093400	12.653156449400	T T T
5.711605317883	7.806056136100	12.653276418700	T T T
7.069849364383	5.452900636000	12.654403428800	T T T
4.354069371283	8.591174586800	10.512295310700	T T T
7.070441365783	7.019948013700	10.514598752600	T T T
7.071576073983	5.452791791300	8.376490163200	T T T
5.713318829483	7.804835074400	8.377821077100	T T T
2.996069013483	7.804498981300	8.378008172900	T T T
0.278603093883	12.511539093400	12.653156449400	T T T
2.994965317883	12.511406136100	12.653276418700	T T T
4.353209364383	10.158250636000	12.654403428800	T T T

1.637429371283	13.296524586800	10.512295310700	T T T
4.353801365783	11.725298013700	10.514598752600	T T T
4.354936073983	10.158141791300	8.376490163200	T T T
2.996678829483	12.510185074400	8.377821077100	T T T
0.279429013483	12.509848981300	8.378008172900	T T T
11.145153093883	3.100839093400	12.653156449400	T T T
13.861515317883	3.100706136100	12.653276418700	T T T
15.219759364383	0.747550636000	12.654403428800	T T T
12.503979371283	3.885824586800	10.512295310700	T T T
15.220351365783	2.314598013700	10.514598752600	T T T
15.221486073983	0.747441791300	8.376490163200	T T T
13.863228829483	3.099485074400	8.377821077100	T T T
11.145979013483	3.099148981300	8.378008172900	T T T
8.428513093883	7.806189093400	12.653156449400	T T T
11.144875317883	7.806056136100	12.653276418700	T T T
12.503119364383	5.452900636000	12.654403428800	T T T
9.787339371283	8.591174586800	10.512295310700	T T T
12.503711365783	7.019948013700	10.514598752600	T T T
12.504846073983	5.452791791300	8.376490163200	T T T
11.146588829483	7.804835074400	8.377821077100	T T T
8.429339013483	7.804498981300	8.378008172900	T T T
5.711873093883	12.511539093400	12.653156449400	T T T
8.428235317883	12.511406136100	12.653276418700	T T T
9.786479364383	10.158250636000	12.654403428800	T T T
7.070699371283	13.296524586800	10.512295310700	T T T
9.787071365783	11.725298013700	10.514598752600	T T T
9.788206073983	10.158141791300	8.376490163200	T T T
8.429948829483	12.510185074400	8.377821077100	T T T
5.712699013483	12.509848981300	8.378008172900	T T T
16.578423093883	3.100839093400	12.653156449400	T T T
19.294785317883	3.100706136100	12.653276418700	T T T
20.653029364383	0.747550636000	12.654403428800	T T T
17.937249371283	3.885824586800	10.512295310700	T T T
20.653621365783	2.314598013700	10.514598752600	T T T
20.654756073983	0.747441791300	8.376490163200	T T T
19.296498829483	3.099485074400	8.377821077100	T T T
16.579249013483	3.099148981300	8.378008172900	T T T
13.861783093883	7.806189093400	12.653156449400	T T T
16.578145317883	7.806056136100	12.653276418700	T T T
17.936389364383	5.452900636000	12.654403428800	T T T
15.220609371283	8.591174586800	10.512295310700	T T T
17.936981365783	7.019948013700	10.514598752600	T T T
17.938116073983	5.452791791300	8.376490163200	T T T
16.579858829483	7.804835074400	8.377821077100	T T T
13.862609013483	7.804498981300	8.378008172900	T T T
11.145143093883	12.511539093400	12.653156449400	T T T
13.861505317883	12.511406136100	12.653276418700	T T T
15.219749364383	10.158250636000	12.654403428800	T T T
12.503969371283	13.296524586800	10.512295310700	T T T
15.220341365783	11.725298013700	10.514598752600	T T T
15.221476073983	10.158141791300	8.376490163200	T T T
13.863218829483	12.510185074400	8.377821077100	T T T
11.145969013483	12.509848981300	8.378008172900	T T T

commentline Fig. 4 – 18th point (0.03 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

0.000000000 0.000000000 24.000000000

Ru Si O

108 36 72

Selective

Cartesian

1.358300000000	2.352700000000	1.000000000000	F	F	F
-1.358300000000	2.352700000000	1.000000000000	F	F	F
2.716600000000	0.000000000000	1.000000000000	F	F	F
0.000000000000	0.000000000000	1.000000000000	F	F	F
1.358300000000	0.784200000000	3.141100000000	F	F	F
4.075000000000	0.784200000000	3.141100000000	F	F	F
0.000000000000	3.136900000000	3.141100000000	F	F	F
2.716600000000	3.136900000000	3.141100000000	F	F	F
1.358312238800	2.352741666300	5.193448999800	T	T	T
4.075112645700	2.353521319700	5.184454391300	T	T	T
0.000204066800	4.705661034200	5.193491229800	T	T	T
2.716589994700	4.705639284500	5.193549923200	T	T	T
-1.358340000000	7.058050000000	1.000000000000	F	F	F
-4.074940000000	7.058050000000	1.000000000000	F	F	F
-0.000040000000	4.705350000000	1.000000000000	F	F	F
-2.716640000000	4.705350000000	1.000000000000	F	F	F
-1.358340000000	5.489550000000	3.141100000000	F	F	F
1.358360000000	5.489550000000	3.141100000000	F	F	F
-2.716640000000	7.842250000000	3.141100000000	F	F	F
-0.000040000000	7.842250000000	3.141100000000	F	F	F
-1.358327761200	7.058091666300	5.193448999800	T	T	T
1.358472645700	7.058871319700	5.184454391300	T	T	T
-2.716435933200	9.411011034200	5.193491229800	T	T	T
-0.000050005300	9.410989284500	5.193549923200	T	T	T
-4.074980000000	11.763400000000	1.000000000000	F	F	F
-6.791580000000	11.763400000000	1.000000000000	F	F	F
-2.716680000000	9.410700000000	1.000000000000	F	F	F
-5.433280000000	9.410700000000	1.000000000000	F	F	F
-4.074980000000	10.194900000000	3.141100000000	F	F	F
-1.358280000000	10.194900000000	3.141100000000	F	F	F
-5.433280000000	12.547600000000	3.141100000000	F	F	F
-2.716680000000	12.547600000000	3.141100000000	F	F	F
-4.074967761200	11.763441666300	5.193448999800	T	T	T
-1.358167354300	11.764221319700	5.184454391300	T	T	T
-5.433075933200	14.116361034200	5.193491229800	T	T	T
-2.716690005300	14.116339284500	5.193549923200	T	T	T
6.791570000000	2.352700000000	1.000000000000	F	F	F
4.074970000000	2.352700000000	1.000000000000	F	F	F
8.149870000000	0.000000000000	1.000000000000	F	F	F
5.433270000000	0.000000000000	1.000000000000	F	F	F
6.791570000000	0.784200000000	3.141100000000	F	F	F
9.508270000000	0.784200000000	3.141100000000	F	F	F
5.433270000000	3.136900000000	3.141100000000	F	F	F
8.149870000000	3.136900000000	3.141100000000	F	F	F
6.791582238800	2.352741666300	5.193448999800	T	T	T
9.508382645700	2.353521319700	5.184454391300	T	T	T
5.433474066800	4.705661034200	5.193491229800	T	T	T
8.149859994700	4.705639284500	5.193549923200	T	T	T
4.074930000000	7.058050000000	1.000000000000	F	F	F

1.358330000000	7.058050000000	1.000000000000	F F F
5.433230000000	4.705350000000	1.000000000000	F F F
2.716630000000	4.705350000000	1.000000000000	F F F
4.074930000000	5.489550000000	3.141100000000	F F F
6.791630000000	5.489550000000	3.141100000000	F F F
2.716630000000	7.842250000000	3.141100000000	F F F
5.433230000000	7.842250000000	3.141100000000	F F F
4.074942238800	7.058091666300	5.193448999800	T T T
6.791742645700	7.058871319700	5.184454391300	T T T
2.716834066800	9.411011034200	5.193491229800	T T T
5.433219994700	9.410989284500	5.193549923200	T T T
1.358290000000	11.763400000000	1.000000000000	F F F
-1.358310000000	11.763400000000	1.000000000000	F F F
2.716590000000	9.410700000000	1.000000000000	F F F
-0.000010000000	9.410700000000	1.000000000000	F F F
1.358290000000	10.194900000000	3.141100000000	F F F
4.074990000000	10.194900000000	3.141100000000	F F F
-0.000010000000	12.547600000000	3.141100000000	F F F
2.716590000000	12.547600000000	3.141100000000	F F F
1.358302238800	11.763441666300	5.193448999800	T T T
4.075102645700	11.764221319700	5.184454391300	T T T
0.000194066800	14.116361034200	5.193491229800	T T T
2.716579994700	14.116339284500	5.193549923200	T T T
12.224840000000	2.352700000000	1.000000000000	F F F
9.508240000000	2.352700000000	1.000000000000	F F F
13.583140000000	0.000000000000	1.000000000000	F F F
10.866540000000	0.000000000000	1.000000000000	F F F
12.224840000000	0.784200000000	3.141100000000	F F F
14.941540000000	0.784200000000	3.141100000000	F F F
10.866540000000	3.136900000000	3.141100000000	F F F
13.583140000000	3.136900000000	3.141100000000	F F F
12.224852238800	2.352741666300	5.193448999800	T T T
14.941652645700	2.353521319700	5.184454391300	T T T
10.866744066800	4.705661034200	5.193491229800	T T T
13.583129994700	4.705639284500	5.193549923200	T T T
9.508200000000	7.058050000000	1.000000000000	F F F
6.791600000000	7.058050000000	1.000000000000	F F F
10.866500000000	4.705350000000	1.000000000000	F F F
8.149900000000	4.705350000000	1.000000000000	F F F
9.508200000000	5.489550000000	3.141100000000	F F F
12.224900000000	5.489550000000	3.141100000000	F F F
8.149900000000	7.842250000000	3.141100000000	F F F
10.866500000000	7.842250000000	3.141100000000	F F F
9.508212238800	7.058091666300	5.193448999800	T T T
12.225012645700	7.058871319700	5.184454391300	T T T
8.150104066800	9.411011034200	5.193491229800	T T T
10.866489994700	9.410989284500	5.193549923200	T T T
6.791560000000	11.763400000000	1.000000000000	F F F
4.074960000000	11.763400000000	1.000000000000	F F F
8.149860000000	9.410700000000	1.000000000000	F F F
5.433260000000	9.410700000000	1.000000000000	F F F
6.791560000000	10.194900000000	3.141100000000	F F F
9.508260000000	10.194900000000	3.141100000000	F F F
5.433260000000	12.547600000000	3.141100000000	F F F
8.149860000000	12.547600000000	3.141100000000	F F F
6.791572238800	11.763441666300	5.193448999800	T T T
9.508372645700	11.764221319700	5.184454391300	T T T
5.433464066800	14.116361034200	5.193491229800	T T T

8.149849994700	14.116339284500	5.193549923200	T T T
11.073552820264	3.884931843200	12.137482891300	T T T
13.790171029264	2.316013296800	12.139605615300	T T T
11.074741731164	3.884195184000	8.888252685300	T T T
13.791328442964	2.315242773000	8.892393552400	T T T
8.356912820264	8.590281843200	12.137482891300	T T T
11.073531029264	7.021363296800	12.139605615300	T T T
8.358101731164	8.589545184000	8.888252685300	T T T
11.074688442964	7.020592773000	8.892393552400	T T T
5.640272820264	13.295631843200	12.137482891300	T T T
8.356891029264	11.726713296800	12.139605615300	T T T
5.641461731164	13.294895184000	8.888252685300	T T T
8.358048442964	11.725942773000	8.892393552400	T T T
16.506822820264	3.884931843200	12.137482891300	T T T
19.223441029264	2.316013296800	12.139605615300	T T T
16.508011731164	3.884195184000	8.888252685300	T T T
19.224598442964	2.315242773000	8.892393552400	T T T
13.790182820264	8.590281843200	12.137482891300	T T T
16.506801029264	7.021363296800	12.139605615300	T T T
13.791371731164	8.589545184000	8.888252685300	T T T
16.507958442964	7.020592773000	8.892393552400	T T T
11.073542820264	13.295631843200	12.137482891300	T T T
13.790161029264	11.726713296800	12.139605615300	T T T
11.074731731164	13.294895184000	8.888252685300	T T T
13.791318442964	11.725942773000	8.892393552400	T T T
21.940092820264	3.884931843200	12.137482891300	T T T
24.656711029264	2.316013296800	12.139605615300	T T T
21.941281731164	3.884195184000	8.888252685300	T T T
24.657868442964	2.315242773000	8.892393552400	T T T
19.223452820264	8.590281843200	12.137482891300	T T T
21.940071029264	7.021363296800	12.139605615300	T T T
19.224641731164	8.589545184000	8.888252685300	T T T
21.941228442964	7.020592773000	8.892393552400	T T T
16.506812820264	13.295631843200	12.137482891300	T T T
19.223431029264	11.726713296800	12.139605615300	T T T
16.508001731164	13.294895184000	8.888252685300	T T T
19.224588442964	11.725942773000	8.892393552400	T T T
9.715344824164	3.100839093400	12.653156449400	T T T
12.431707048164	3.100706136100	12.653276418700	T T T
13.789951094664	0.747550636000	12.654403428800	T T T
11.074171101564	3.885824586800	10.512295310700	T T T
13.790543096064	2.314598013700	10.514598752600	T T T
13.791677804264	0.747441791300	8.376490163200	T T T
12.433420559764	3.099485074400	8.377821077100	T T T
9.716170743764	3.099148981300	8.378008172900	T T T
6.998704824164	7.806189093400	12.653156449400	T T T
9.715067048164	7.806056136100	12.653276418700	T T T
11.073311094664	5.452900636000	12.654403428800	T T T
8.357531101564	8.591174586800	10.512295310700	T T T
11.073903096064	7.019948013700	10.514598752600	T T T
11.075037804264	5.452791791300	8.376490163200	T T T
9.716780559764	7.804835074400	8.377821077100	T T T
6.999530743764	7.804498981300	8.378008172900	T T T
4.282064824164	12.511539093400	12.653156449400	T T T
6.998427048164	12.511406136100	12.653276418700	T T T
8.356671094664	10.158250636000	12.654403428800	T T T
5.640891101564	13.296524586800	10.512295310700	T T T
8.357263096064	11.725298013700	10.514598752600	T T T

8.358397804264	10.158141791300	8.376490163200	T T T
7.000140559764	12.510185074400	8.377821077100	T T T
4.282890743764	12.509848981300	8.378008172900	T T T
15.148614824164	3.100839093400	12.653156449400	T T T
17.864977048164	3.100706136100	12.653276418700	T T T
19.223221094664	0.747550636000	12.654403428800	T T T
16.507441101564	3.885824586800	10.512295310700	T T T
19.223813096064	2.314598013700	10.514598752600	T T T
19.224947804264	0.747441791300	8.376490163200	T T T
17.866690559764	3.099485074400	8.377821077100	T T T
15.149440743764	3.099148981300	8.378008172900	T T T
12.431974824164	7.806189093400	12.653156449400	T T T
15.148337048164	7.806056136100	12.653276418700	T T T
16.506581094664	5.452900636000	12.654403428800	T T T
13.790801101564	8.591174586800	10.512295310700	T T T
16.507173096064	7.019948013700	10.514598752600	T T T
16.508307804264	5.452791791300	8.376490163200	T T T
15.150050559764	7.804835074400	8.377821077100	T T T
12.432800743764	7.804498981300	8.378008172900	T T T
9.715334824164	12.511539093400	12.653156449400	T T T
12.431697048164	12.511406136100	12.653276418700	T T T
13.789941094664	10.158250636000	12.654403428800	T T T
11.074161101564	13.296524586800	10.512295310700	T T T
13.790533096064	11.725298013700	10.514598752600	T T T
13.791667804264	10.158141791300	8.376490163200	T T T
12.433410559764	12.510185074400	8.377821077100	T T T
9.716160743764	12.509848981300	8.378008172900	T T T
20.581884824164	3.100839093400	12.653156449400	T T T
23.298247048164	3.100706136100	12.653276418700	T T T
24.656491094664	0.747550636000	12.654403428800	T T T
21.940711101564	3.885824586800	10.512295310700	T T T
24.657083096064	2.314598013700	10.514598752600	T T T
24.658217804264	0.747441791300	8.376490163200	T T T
23.299960559764	3.099485074400	8.377821077100	T T T
20.582710743764	3.099148981300	8.378008172900	T T T
17.865244824164	7.806189093400	12.653156449400	T T T
20.581607048164	7.806056136100	12.653276418700	T T T
21.939851094664	5.452900636000	12.654403428800	T T T
19.224071101564	8.591174586800	10.512295310700	T T T
21.940443096064	7.019948013700	10.514598752600	T T T
21.941577804264	5.452791791300	8.376490163200	T T T
20.583320559764	7.804835074400	8.377821077100	T T T
17.866070743764	7.804498981300	8.378008172900	T T T
15.148604824164	12.511539093400	12.653156449400	T T T
17.864967048164	12.511406136100	12.653276418700	T T T
19.223211094664	10.158250636000	12.654403428800	T T T
16.507431101564	13.296524586800	10.512295310700	T T T
19.223803096064	11.725298013700	10.514598752600	T T T
19.224937804264	10.158141791300	8.376490163200	T T T
17.866680559764	12.510185074400	8.377821077100	T T T
15.149430743764	12.509848981300	8.378008172900	T T T

11.2. The 1O-(2x2) Ru(0001) Substrate

Commentline: Fig. 5 – 1st point (0.02 eV)

1.0

+16.2998100000 +0.0000000000 +0.0000000000

-8.1499200000 +14.1160500000 +0.0000000000

+0.0000000000 +0.0000000000 +24.0000000000

Ru Si O Os

108 36 72 9

Selective

Cartesian

+1.3583000000 +2.3527000000 +1.0000000000 F F F

-1.3583000000 +2.3527000000 +1.0000000000 F F F

+2.7166000000 +0.0000000000 +1.0000000000 F F F

+0.0000000000 +0.0000000000 +1.0000000000 F F F

+1.3583000000 +0.7842000000 +3.1411000000 F F F

+4.0750000000 +0.7842000000 +3.1411000000 F F F

+0.0000000000 +3.1369000000 +3.1411000000 F F F

+2.7166000000 +3.1369000000 +3.1411000000 F F F

+1.3560585876 +2.4547507619 +5.2366561353 T T T

+4.0727961767 +2.3521335698 +5.1720686855 T T T

+0.0867350197 +4.6531531246 +5.2363819785 T T T

+2.6238665338 +4.6521819914 +5.2372994561 T T T

-1.3583400000 +7.0580500000 +1.0000000000 F F F

-4.0749400000 +7.0580500000 +1.0000000000 F F F

-0.0000400000 +4.7053500000 +1.0000000000 F F F

-2.7166400000 +4.7053500000 +1.0000000000 F F F

-1.3583400000 +5.4895500000 +3.1411000000 F F F

+1.3583600000 +5.4895500000 +3.1411000000 F F F

-2.7166400000 +7.8422500000 +3.1411000000 F F F

-0.0000400000 +7.8422500000 +3.1411000000 F F F

-1.3605814124 +7.1601007619 +5.2366561353 T T T

+1.3561561767 +7.0574835698 +5.1720686855 T T T

-2.6299049803 +9.3585031246 +5.2363819785 T T T

-0.0927734662 +9.3575319914 +5.2372994561 T T T

-4.0749800000 +11.7634000000 +1.0000000000 F F F

-6.7915800000 +11.7634000000 +1.0000000000 F F F

-2.7166800000 +9.4107000000 +1.0000000000 F F F

-5.4332800000 +9.4107000000 +1.0000000000 F F F

-4.0749800000 +10.1949000000 +3.1411000000 F F F

-1.3582800000 +10.1949000000 +3.1411000000 F F F

-5.4332800000 +12.5476000000 +3.1411000000 F F F

-2.7166800000 +12.5476000000 +3.1411000000 F F F

-4.0772214124 +11.8654507619 +5.2366561353 T T T

-1.3604838233 +11.7628335698 +5.1720686855 T T T

-5.3465449803 +14.0638531246 +5.2363819785 T T T

-2.8094134662 +14.0628819914 +5.2372994561 T T T

+6.7915700000 +2.3527000000 +1.0000000000 F F F

+4.0749700000 +2.3527000000 +1.0000000000 F F F

+8.1498700000 +0.0000000000 +1.0000000000 F F F

+5.4332700000 +0.0000000000 +1.0000000000 F F F

+6.7915700000 +0.7842000000 +3.1411000000 F F F

+9.5082700000 +0.7842000000 +3.1411000000 F F F

+5.4332700000 +3.1369000000 +3.1411000000 F F F

+8.1498700000 +3.1369000000 +3.1411000000 F F F

+6.7893285876 +2.4547507619 +5.2366561353 T T T

+9.5060661767 +2.3521335698 +5.1720686855 T T T
 +5.5200050197 +4.6531531246 +5.2363819785 T T T
 +8.0571365338 +4.6521819914 +5.2372994561 T T T
 +4.0749300000 +7.0580500000 +1.0000000000 F F F
 +1.3583300000 +7.0580500000 +1.0000000000 F F F
 +5.4332300000 +4.7053500000 +1.0000000000 F F F
 +2.7166300000 +4.7053500000 +1.0000000000 F F F
 +4.0749300000 +5.4895500000 +3.1411000000 F F F
 +6.7916300000 +5.4895500000 +3.1411000000 F F F
 +2.7166300000 +7.8422500000 +3.1411000000 F F F
 +5.4332300000 +7.8422500000 +3.1411000000 F F F
 +4.0726885876 +7.1601007619 +5.2366561353 T T T
 +6.7894261767 +7.0574835698 +5.1720686855 T T T
 +2.8033650197 +9.3585031246 +5.2363819785 T T T
 +5.3404965338 +9.3575319914 +5.2372994561 T T T
 +1.3582900000 +11.7634000000 +1.0000000000 F F F
 -1.3583100000 +11.7634000000 +1.0000000000 F F F
 +2.7165900000 +9.4107000000 +1.0000000000 F F F
 -0.0000100000 +9.4107000000 +1.0000000000 F F F
 +1.3582900000 +10.1949000000 +3.1411000000 F F F
 +4.0749900000 +10.1949000000 +3.1411000000 F F F
 -0.0000100000 +12.5476000000 +3.1411000000 F F F
 +2.7165900000 +12.5476000000 +3.1411000000 F F F
 +1.3560485876 +11.8654507619 +5.2366561353 T T T
 +4.0727861767 +11.7628335698 +5.1720686855 T T T
 +0.0867250197 +14.0638531246 +5.2363819785 T T T
 +2.6238565338 +14.0628819914 +5.2372994561 T T T
 +12.2248400000 +2.3527000000 +1.0000000000 F F F
 +9.5082400000 +2.3527000000 +1.0000000000 F F F
 +13.5831400000 +0.0000000000 +1.0000000000 F F F
 +10.8665400000 +0.0000000000 +1.0000000000 F F F
 +12.2248400000 +0.7842000000 +3.1411000000 F F F
 +14.9415400000 +0.7842000000 +3.1411000000 F F F
 +10.8665400000 +3.1369000000 +3.1411000000 F F F
 +13.5831400000 +3.1369000000 +3.1411000000 F F F
 +12.2225985876 +2.4547507619 +5.2366561353 T T T
 +14.9393361767 +2.3521335698 +5.1720686855 T T T
 +10.9532750197 +4.6531531246 +5.2363819785 T T T
 +13.4904065338 +4.6521819914 +5.2372994561 T T T
 +9.5082000000 +7.0580500000 +1.0000000000 F F F
 +6.7916000000 +7.0580500000 +1.0000000000 F F F
 +10.8665000000 +4.7053500000 +1.0000000000 F F F
 +8.1499000000 +4.7053500000 +1.0000000000 F F F
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 +12.2249000000 +5.4895500000 +3.1411000000 F F F
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 +10.8665000000 +7.8422500000 +3.1411000000 F F F
 +9.5059585876 +7.1601007619 +5.2366561353 T T T
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 +4.0749600000 +11.7634000000 +1.0000000000 F F F
 +8.1498600000 +9.4107000000 +1.0000000000 F F F
 +5.4332600000 +9.4107000000 +1.0000000000 F F F
 +6.7915600000 +10.1949000000 +3.1411000000 F F F
 +9.5082600000 +10.1949000000 +3.1411000000 F F F
 +5.4332600000 +12.5476000000 +3.1411000000 F F F

+8.1498600000 +12.5476000000 +3.1411000000 F F F
 +6.7893185876 +11.8654507619 +5.2366561353 T T T
 +9.5060561767 +11.7628335698 +5.1720686855 T T T
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 +1.3587157416 +3.8880664569 +12.3781886397 T T T
 +4.0764908067 +2.3227355843 +12.3824107959 T T T
 +1.3450177077 +3.8813208704 +9.1252699292 T T T
 +4.0627995434 +2.3158718390 +9.1334320442 T T T
 -1.3579242584 +8.5934164569 +12.3781886397 T T T
 +1.3598508067 +7.0280855843 +12.3824107959 T T T
 -1.3716222923 +8.5866708704 +9.1252699292 T T T
 +1.3461595434 +7.0212218390 +9.1334320442 T T T
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 -4.0882622923 +13.2920208704 +9.1252699292 T T T
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 -4.0783278698 +10.1929289773 +6.3822465352 F F F

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commentline Fig. 5 – 5th point (1.52 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

0.000000000 0.000000000 24.000000000

Ru Si O Os

108 36 72 9

Selective

Cartesian

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0.000000000000 0.000000000000 1.000000000000 F F F
1.358300000000 0.784200000000 3.141100000000 F F F
4.075000000000 0.784200000000 3.141100000000 F F F
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4.072796176700 2.352133569800 5.172068685500 T T T
0.086735019700 4.653153124600 5.236381978500 T T T
2.623866533800 4.652181991400 5.237299456100 T T T
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-2.716640000000 4.705350000000 1.000000000000 F F F
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-6.791580000000 11.763400000000 1.000000000000 F F F
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4.074970000000 2.352700000000 1.000000000000 F F F

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7.787939419301	12.726321775181	10.756907565600	T	T	T
7.772419182001	11.148925787581	8.618075143800	T	T	T
6.424739845701	13.502151881481	8.611769489700	T	T	T
3.705652226601	13.495083262481	8.608282602500	T	T	T
1.354952130200	0.782228977300	6.382246535200	F	F	F
-1.361687869800	5.487578977300	6.382246535200	F	F	F
-4.078327869800	10.192928977300	6.382246535200	F	F	F
6.788222130200	0.782228977300	6.382246535200	F	F	F
4.071582130200	5.487578977300	6.382246535200	F	F	F
1.354942130200	10.192928977300	6.382246535200	F	F	F
12.221492130200	0.782228977300	6.382246535200	F	F	F
9.504852130200	5.487578977300	6.382246535200	F	F	F
6.788212130200	10.192928977300	6.382246535200	F	F	F

commentline Fig. 5 – 11th point (4.11 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

0.000000000 0.000000000 24.000000000

Ru Si O Os

108 36 72 9

Selective

Cartesian

1.358300000000	2.352700000000	1.000000000000	F	F	F
-1.358300000000	2.352700000000	1.000000000000	F	F	F
2.716600000000	0.000000000000	1.000000000000	F	F	F
0.000000000000	0.000000000000	1.000000000000	F	F	F
1.358300000000	0.784200000000	3.141100000000	F	F	F
4.075000000000	0.784200000000	3.141100000000	F	F	F
0.000000000000	3.136900000000	3.141100000000	F	F	F
2.716600000000	3.136900000000	3.141100000000	F	F	F
1.356058587600	2.454750761900	5.236656135300	T	T	T
4.072796176700	2.352133569800	5.172068685500	T	T	T
0.086735019700	4.653153124600	5.236381978500	T	T	T
2.623866533800	4.652181991400	5.237299456100	T	T	T
-1.358340000000	7.058050000000	1.000000000000	F	F	F
-4.074940000000	7.058050000000	1.000000000000	F	F	F
-0.000040000000	4.705350000000	1.000000000000	F	F	F
-2.716640000000	4.705350000000	1.000000000000	F	F	F
-1.358340000000	5.489550000000	3.141100000000	F	F	F
1.358360000000	5.489550000000	3.141100000000	F	F	F
-2.716640000000	7.842250000000	3.141100000000	F	F	F
-0.000040000000	7.842250000000	3.141100000000	F	F	F
-1.360581412400	7.160100761900	5.236656135300	T	T	T
1.356156176700	7.057483569800	5.172068685500	T	T	T
-2.629904980300	9.358503124600	5.236381978500	T	T	T
-0.092773466200	9.357531991400	5.237299456100	T	T	T
-4.074980000000	11.763400000000	1.000000000000	F	F	F
-6.791580000000	11.763400000000	1.000000000000	F	F	F
-2.716680000000	9.410700000000	1.000000000000	F	F	F
-5.433280000000	9.410700000000	1.000000000000	F	F	F
-4.074980000000	10.194900000000	3.141100000000	F	F	F
-1.358280000000	10.194900000000	3.141100000000	F	F	F
-5.433280000000	12.547600000000	3.141100000000	F	F	F

-2.716680000000	12.547600000000	3.141100000000	F F F
-4.077221412400	11.865450761900	5.236656135300	T T T
-1.360483823300	11.762833569800	5.172068685500	T T T
-5.346544980300	14.063853124600	5.236381978500	T T T
-2.809413466200	14.062881991400	5.237299456100	T T T
6.791570000000	2.352700000000	1.000000000000	F F F
4.074970000000	2.352700000000	1.000000000000	F F F
8.149870000000	0.000000000000	1.000000000000	F F F
5.433270000000	0.000000000000	1.000000000000	F F F
6.791570000000	0.784200000000	3.141100000000	F F F
9.508270000000	0.784200000000	3.141100000000	F F F
5.433270000000	3.136900000000	3.141100000000	F F F
8.149870000000	3.136900000000	3.141100000000	F F F
6.789328587600	2.454750761900	5.236656135300	T T T
9.506066176700	2.352133569800	5.172068685500	T T T
5.520005019700	4.653153124600	5.236381978500	T T T
8.057136533800	4.652181991400	5.237299456100	T T T
4.074930000000	7.058050000000	1.000000000000	F F F
1.358330000000	7.058050000000	1.000000000000	F F F
5.433230000000	4.705350000000	1.000000000000	F F F
2.716630000000	4.705350000000	1.000000000000	F F F
4.074930000000	5.489550000000	3.141100000000	F F F
6.791630000000	5.489550000000	3.141100000000	F F F
2.716630000000	7.842250000000	3.141100000000	F F F
5.433230000000	7.842250000000	3.141100000000	F F F
4.072688587600	7.160100761900	5.236656135300	T T T
6.789426176700	7.057483569800	5.172068685500	T T T
2.803365019700	9.358503124600	5.236381978500	T T T
5.340496533800	9.357531991400	5.237299456100	T T T
1.358290000000	11.763400000000	1.000000000000	F F F
-1.358310000000	11.763400000000	1.000000000000	F F F
2.716590000000	9.410700000000	1.000000000000	F F F
-0.000010000000	9.410700000000	1.000000000000	F F F
1.358290000000	10.194900000000	3.141100000000	F F F
4.074990000000	10.194900000000	3.141100000000	F F F
-0.000010000000	12.547600000000	3.141100000000	F F F
2.716590000000	12.547600000000	3.141100000000	F F F
1.356048587600	11.865450761900	5.236656135300	T T T
4.072786176700	11.762833569800	5.172068685500	T T T
0.086725019700	14.063853124600	5.236381978500	T T T
2.623856533800	14.062881991400	5.237299456100	T T T
12.224840000000	2.352700000000	1.000000000000	F F F
9.508240000000	2.352700000000	1.000000000000	F F F
13.583140000000	0.000000000000	1.000000000000	F F F
10.866540000000	0.000000000000	1.000000000000	F F F
12.224840000000	0.784200000000	3.141100000000	F F F
14.941540000000	0.784200000000	3.141100000000	F F F
10.866540000000	3.136900000000	3.141100000000	F F F
13.583140000000	3.136900000000	3.141100000000	F F F
12.222598587600	2.454750761900	5.236656135300	T T T
14.939336176700	2.352133569800	5.172068685500	T T T
10.953275019700	4.653153124600	5.236381978500	T T T
13.490406533800	4.652181991400	5.237299456100	T T T
9.508200000000	7.058050000000	1.000000000000	F F F
6.791600000000	7.058050000000	1.000000000000	F F F
10.866500000000	4.705350000000	1.000000000000	F F F
8.149900000000	4.705350000000	1.000000000000	F F F
9.508200000000	5.489550000000	3.141100000000	F F F

12.224900000000	5.489550000000	3.141100000000	F F F
8.149900000000	7.842250000000	3.141100000000	F F F
10.866500000000	7.842250000000	3.141100000000	F F F
9.505958587600	7.160100761900	5.236656135300	T T T
12.222696176700	7.057483569800	5.172068685500	T T T
8.236635019700	9.358503124600	5.236381978500	T T T
10.773766533800	9.357531991400	5.237299456100	T T T
6.791560000000	11.763400000000	1.000000000000	F F F
4.074960000000	11.763400000000	1.000000000000	F F F
8.149860000000	9.410700000000	1.000000000000	F F F
5.433260000000	9.410700000000	1.000000000000	F F F
6.791560000000	10.194900000000	3.141100000000	F F F
9.508260000000	10.194900000000	3.141100000000	F F F
5.433260000000	12.547600000000	3.141100000000	F F F
8.149860000000	12.547600000000	3.141100000000	F F F
6.789318587600	11.865450761900	5.236656135300	T T T
9.506056176700	11.762833569800	5.172068685500	T T T
5.519995019700	14.063853124600	5.236381978500	T T T
8.057126533800	14.062881991400	5.237299456100	T T T
-2.930710727591	6.364566545467	12.378188639700	T T T
-0.212935662491	4.799235672867	12.382410795900	T T T
-2.944408761491	6.357820958967	9.125269929200	T T T
-0.226626925791	4.792371927567	9.133432044200	T T T
-5.647350727591	11.069916545467	12.378188639700	T T T
-2.929575662491	9.504585672867	12.382410795900	T T T
-5.661048761491	11.063170958967	9.125269929200	T T T
-2.943266925791	9.497721927567	9.133432044200	T T T
-8.363990727591	15.775266545467	12.378188639700	T T T
-5.646215662491	14.209935672867	12.382410795900	T T T
-8.377688761491	15.768520958967	9.125269929200	T T T
-5.659906925791	14.203071927567	9.133432044200	T T T
2.502559272409	6.364566545467	12.378188639700	T T T
5.220334337509	4.799235672867	12.382410795900	T T T
2.488861238509	6.357820958967	9.125269929200	T T T
5.206643074209	4.792371927567	9.133432044200	T T T
-0.214080727591	11.069916545467	12.378188639700	T T T
2.503694337509	9.504585672867	12.382410795900	T T T
-0.227778761491	11.063170958967	9.125269929200	T T T
2.490003074209	9.497721927567	9.133432044200	T T T
-2.930720727591	15.775266545467	12.378188639700	T T T
-0.212945662491	14.209935672867	12.382410795900	T T T
-2.944418761491	15.768520958967	9.125269929200	T T T
-0.226636925791	14.203071927567	9.133432044200	T T T
7.935829272409	6.364566545467	12.378188639700	T T T
10.653604337509	4.799235672867	12.382410795900	T T T
7.922131238509	6.357820958967	9.125269929200	T T T
10.639913074209	4.792371927567	9.133432044200	T T T
5.219189272409	11.069916545467	12.378188639700	T T T
7.936964337509	9.504585672867	12.382410795900	T T T
5.205491238509	11.063170958967	9.125269929200	T T T
7.923273074209	9.497721927567	9.133432044200	T T T
2.502549272409	15.775266545467	12.378188639700	T T T
5.220324337509	14.209935672867	12.382410795900	T T T
2.488851238509	15.768520958967	9.125269929200	T T T
5.206633074209	14.203071927567	9.133432044200	T T T
-4.288116641691	5.582229072867	12.902103536300	T T T
-1.570832386291	5.584616701067	12.898781879500	T T T
-0.209866746691	3.228697199567	12.892684777200	T T T

-2.941698476391	6.353359941167	10.751944326600	T T T
-0.218976510791	4.801521856367	10.756907565600	T T T
-0.234496748091	3.224125868767	8.618075143800	T T T
-1.582176084391	5.577351962667	8.611769489700	T T T
-4.301263703491	5.570283343667	8.608282602500	T T T
-7.004756641691	10.287579072867	12.902103536300	T T T
-4.287472386291	10.289966701067	12.898781879500	T T T
-2.926506746691	7.934047199567	12.892684777200	T T T
-5.658338476391	11.058709941167	10.751944326600	T T T
-2.935616510791	9.506871856367	10.756907565600	T T T
-2.951136748091	7.929475868767	8.618075143800	T T T
-4.298816084391	10.282701962667	8.611769489700	T T T
-7.017903703491	10.275633343667	8.608282602500	T T T
-9.721396641691	14.992929072867	12.902103536300	T T T
-7.004112386291	14.995316701067	12.898781879500	T T T
-5.643146746691	12.639397199567	12.892684777200	T T T
-8.374978476391	15.764059941167	10.751944326600	T T T
-5.652256510791	14.212221856367	10.756907565600	T T T
-5.667776748091	12.634825868767	8.618075143800	T T T
-7.015456084391	14.988051962667	8.611769489700	T T T
-9.734543703491	14.980983343667	8.608282602500	T T T
1.145153358309	5.582229072867	12.902103536300	T T T
3.862437613709	5.584616701067	12.898781879500	T T T
5.223403253309	3.228697199567	12.892684777200	T T T
2.491571523609	6.353359941167	10.751944326600	T T T
5.214293489209	4.801521856367	10.756907565600	T T T
5.198773251909	3.224125868767	8.618075143800	T T T
3.851093915609	5.577351962667	8.611769489700	T T T
1.132006296509	5.570283343667	8.608282602500	T T T
-1.571486641691	10.287579072867	12.902103536300	T T T
1.145797613709	10.289966701067	12.898781879500	T T T
2.506763253309	7.934047199567	12.892684777200	T T T
-0.225068476391	11.058709941167	10.751944326600	T T T
2.497653489209	9.506871856367	10.756907565600	T T T
2.482133251909	7.929475868767	8.618075143800	T T T
1.134453915609	10.282701962667	8.611769489700	T T T
-1.584633703491	10.275633343667	8.608282602500	T T T
-4.288126641691	14.992929072867	12.902103536300	T T T
-1.570842386291	14.995316701067	12.898781879500	T T T
-0.209876746691	12.639397199567	12.892684777200	T T T
-2.941708476391	15.764059941167	10.751944326600	T T T
-0.218986510791	14.212221856367	10.756907565600	T T T
-0.234506748091	12.634825868767	8.618075143800	T T T
-1.582186084391	14.988051962667	8.611769489700	T T T
-4.301273703491	14.980983343667	8.608282602500	T T T
6.578423358309	5.582229072867	12.902103536300	T T T
9.295707613709	5.584616701067	12.898781879500	T T T
10.656673253309	3.228697199567	12.892684777200	T T T
7.924841523609	6.353359941167	10.751944326600	T T T
10.647563489209	4.801521856367	10.756907565600	T T T
10.632043251909	3.224125868767	8.618075143800	T T T
9.284363915609	5.577351962667	8.611769489700	T T T
6.565276296509	5.570283343667	8.608282602500	T T T
3.861783358309	10.287579072867	12.902103536300	T T T
6.579067613709	10.289966701067	12.898781879500	T T T
7.940033253309	7.934047199567	12.892684777200	T T T
5.208201523609	11.058709941167	10.751944326600	T T T
7.930923489209	9.506871856367	10.756907565600	T T T

7.915403251909	7.929475868767	8.618075143800	T	T	T
6.567723915609	10.282701962667	8.611769489700	T	T	T
3.848636296509	10.275633343667	8.608282602500	T	T	T
1.145143358309	14.992929072867	12.902103536300	T	T	T
3.862427613709	14.995316701067	12.898781879500	T	T	T
5.223393253309	12.639397199567	12.892684777200	T	T	T
2.491561523609	15.764059941167	10.751944326600	T	T	T
5.214283489209	14.212221856367	10.756907565600	T	T	T
5.198763251909	12.634825868767	8.618075143800	T	T	T
3.851083915609	14.988051962667	8.611769489700	T	T	T
1.131996296509	14.980983343667	8.608282602500	T	T	T
1.354952130200	0.782228977300	6.382246535200	F	F	F
-1.361687869800	5.487578977300	6.382246535200	F	F	F
-4.078327869800	10.192928977300	6.382246535200	F	F	F
6.788222130200	0.782228977300	6.382246535200	F	F	F
4.071582130200	5.487578977300	6.382246535200	F	F	F
1.354942130200	10.192928977300	6.382246535200	F	F	F
12.221492130200	0.782228977300	6.382246535200	F	F	F
9.504852130200	5.487578977300	6.382246535200	F	F	F
6.788212130200	10.192928977300	6.382246535200	F	F	F

commentline Fig. 5 – 14th point (0.87 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

0.000000000 0.000000000 24.000000000

Ru Si O Os

108 36 72 9

Selective

Cartesian

1.358300000000	2.352700000000	1.000000000000	F	F	F
-1.358300000000	2.352700000000	1.000000000000	F	F	F
2.716600000000	0.000000000000	1.000000000000	F	F	F
0.000000000000	0.000000000000	1.000000000000	F	F	F
1.358300000000	0.784200000000	3.141100000000	F	F	F
4.075000000000	0.784200000000	3.141100000000	F	F	F
0.000000000000	3.136900000000	3.141100000000	F	F	F
2.716600000000	3.136900000000	3.141100000000	F	F	F
1.356058587600	2.454750761900	5.236656135300	T	T	T
4.072796176700	2.352133569800	5.172068685500	T	T	T
0.086735019700	4.653153124600	5.236381978500	T	T	T
2.623866533800	4.652181991400	5.237299456100	T	T	T
-1.358340000000	7.058050000000	1.000000000000	F	F	F
-4.074940000000	7.058050000000	1.000000000000	F	F	F
-0.000040000000	4.705350000000	1.000000000000	F	F	F
-2.716640000000	4.705350000000	1.000000000000	F	F	F
-1.358340000000	5.489550000000	3.141100000000	F	F	F
1.358360000000	5.489550000000	3.141100000000	F	F	F
-2.716640000000	7.842250000000	3.141100000000	F	F	F
-0.000040000000	7.842250000000	3.141100000000	F	F	F
-1.360581412400	7.160100761900	5.236656135300	T	T	T
1.356156176700	7.057483569800	5.172068685500	T	T	T
-2.629904980300	9.358503124600	5.236381978500	T	T	T
-0.092773466200	9.357531991400	5.237299456100	T	T	T

-4.074980000000	11.763400000000	1.000000000000	F F F
-6.791580000000	11.763400000000	1.000000000000	F F F
-2.716680000000	9.410700000000	1.000000000000	F F F
-5.433280000000	9.410700000000	1.000000000000	F F F
-4.074980000000	10.194900000000	3.141100000000	F F F
-1.358280000000	10.194900000000	3.141100000000	F F F
-5.433280000000	12.547600000000	3.141100000000	F F F
-2.716680000000	12.547600000000	3.141100000000	F F F
-4.077221412400	11.865450761900	5.236656135300	T T T
-1.360483823300	11.762833569800	5.172068685500	T T T
-5.346544980300	14.063853124600	5.236381978500	T T T
-2.809413466200	14.062881991400	5.237299456100	T T T
6.791570000000	2.352700000000	1.000000000000	F F F
4.074970000000	2.352700000000	1.000000000000	F F F
8.149870000000	0.000000000000	1.000000000000	F F F
5.433270000000	0.000000000000	1.000000000000	F F F
6.791570000000	0.784200000000	3.141100000000	F F F
9.508270000000	0.784200000000	3.141100000000	F F F
5.433270000000	3.136900000000	3.141100000000	F F F
8.149870000000	3.136900000000	3.141100000000	F F F
6.789328587600	2.454750761900	5.236656135300	T T T
9.506066176700	2.352133569800	5.172068685500	T T T
5.520005019700	4.653153124600	5.236381978500	T T T
8.057136533800	4.652181991400	5.237299456100	T T T
4.074930000000	7.058050000000	1.000000000000	F F F
1.358330000000	7.058050000000	1.000000000000	F F F
5.433230000000	4.705350000000	1.000000000000	F F F
2.716630000000	4.705350000000	1.000000000000	F F F
4.074930000000	5.489550000000	3.141100000000	F F F
6.791630000000	5.489550000000	3.141100000000	F F F
2.716630000000	7.842250000000	3.141100000000	F F F
5.433230000000	7.842250000000	3.141100000000	F F F
4.072688587600	7.160100761900	5.236656135300	T T T
6.789426176700	7.057483569800	5.172068685500	T T T
2.803365019700	9.358503124600	5.236381978500	T T T
5.340496533800	9.357531991400	5.237299456100	T T T
1.358290000000	11.763400000000	1.000000000000	F F F
-1.358310000000	11.763400000000	1.000000000000	F F F
2.716590000000	9.410700000000	1.000000000000	F F F
-0.000010000000	9.410700000000	1.000000000000	F F F
1.358290000000	10.194900000000	3.141100000000	F F F
4.074990000000	10.194900000000	3.141100000000	F F F
-0.000010000000	12.547600000000	3.141100000000	F F F
2.716590000000	12.547600000000	3.141100000000	F F F
1.356048587600	11.865450761900	5.236656135300	T T T
4.072786176700	11.762833569800	5.172068685500	T T T
0.086725019700	14.063853124600	5.236381978500	T T T
2.623856533800	14.062881991400	5.237299456100	T T T
12.224840000000	2.352700000000	1.000000000000	F F F
9.508240000000	2.352700000000	1.000000000000	F F F
13.583140000000	0.000000000000	1.000000000000	F F F
10.866540000000	0.000000000000	1.000000000000	F F F
12.224840000000	0.784200000000	3.141100000000	F F F
14.941540000000	0.784200000000	3.141100000000	F F F
10.866540000000	3.136900000000	3.141100000000	F F F
13.583140000000	3.136900000000	3.141100000000	F F F
12.222598587600	2.454750761900	5.236656135300	T T T
14.939336176700	2.352133569800	5.172068685500	T T T

10.953275019700	4.653153124600	5.236381978500	T T T
13.490406533800	4.652181991400	5.237299456100	T T T
9.508200000000	7.058050000000	1.000000000000	F F F
6.791600000000	7.058050000000	1.000000000000	F F F
10.866500000000	4.705350000000	1.000000000000	F F F
8.149900000000	4.705350000000	1.000000000000	F F F
9.508200000000	5.489550000000	3.141100000000	F F F
12.224900000000	5.489550000000	3.141100000000	F F F
8.149900000000	7.842250000000	3.141100000000	F F F
10.866500000000	7.842250000000	3.141100000000	F F F
9.505958587600	7.160100761900	5.236656135300	T T T
12.222696176700	7.057483569800	5.172068685500	T T T
8.236635019700	9.358503124600	5.236381978500	T T T
10.773766533800	9.357531991400	5.237299456100	T T T
6.791560000000	11.763400000000	1.000000000000	F F F
4.074960000000	11.763400000000	1.000000000000	F F F
8.149860000000	9.410700000000	1.000000000000	F F F
5.433260000000	9.410700000000	1.000000000000	F F F
6.791560000000	10.194900000000	3.141100000000	F F F
9.508260000000	10.194900000000	3.141100000000	F F F
5.433260000000	12.547600000000	3.141100000000	F F F
8.149860000000	12.547600000000	3.141100000000	F F F
6.789318587600	11.865450761900	5.236656135300	T T T
9.506056176700	11.762833569800	5.172068685500	T T T
5.519995019700	14.063853124600	5.236381978500	T T T
8.057126533800	14.062881991400	5.237299456100	T T T
-4.217538571194	7.107516515944	12.378188639700	T T T
-1.499763506094	5.542185643344	12.382410795900	T T T
-4.231236605094	7.100770929444	9.125269929200	T T T
-1.513454769394	5.535321898044	9.133432044200	T T T
-6.934178571194	11.812866515944	12.378188639700	T T T
-4.216403506094	10.247535643344	12.382410795900	T T T
-6.947876605094	11.806120929444	9.125269929200	T T T
-4.230094769394	10.240671898044	9.133432044200	T T T
-9.650818571194	16.518216515944	12.378188639700	T T T
-6.933043506094	14.952885643344	12.382410795900	T T T
-9.664516605094	16.511470929444	9.125269929200	T T T
-6.946734769394	14.946021898044	9.133432044200	T T T
1.215731428806	7.107516515944	12.378188639700	T T T
3.933506493906	5.542185643344	12.382410795900	T T T
1.202033394906	7.100770929444	9.125269929200	T T T
3.919815230606	5.535321898044	9.133432044200	T T T
-1.500908571194	11.812866515944	12.378188639700	T T T
1.216866493906	10.247535643344	12.382410795900	T T T
-1.514606605094	11.806120929444	9.125269929200	T T T
1.203175230606	10.240671898044	9.133432044200	T T T
-4.217548571194	16.518216515944	12.378188639700	T T T
-1.499773506094	14.952885643344	12.382410795900	T T T
-4.231246605094	16.511470929444	9.125269929200	T T T
-1.513464769394	14.946021898044	9.133432044200	T T T
6.649001428806	7.107516515944	12.378188639700	T T T
9.366776493906	5.542185643344	12.382410795900	T T T
6.635303394906	7.100770929444	9.125269929200	T T T
9.353085230606	5.535321898044	9.133432044200	T T T
3.932361428806	11.812866515944	12.378188639700	T T T
6.650136493906	10.247535643344	12.382410795900	T T T
3.918663394906	11.806120929444	9.125269929200	T T T
6.636445230606	10.240671898044	9.133432044200	T T T

1.215721428806	16.518216515944	12.378188639700	T T T
3.933496493906	14.952885643344	12.382410795900	T T T
1.202023394906	16.511470929444	9.125269929200	T T T
3.919805230606	14.946021898044	9.133432044200	T T T
-5.574944485294	6.325179043344	12.902103536300	T T T
-2.857660229894	6.327566671544	12.898781879500	T T T
-1.496694590294	3.971647170044	12.892684777200	T T T
-4.228526319994	7.096309911644	10.751944326600	T T T
-1.505804354394	5.544471826844	10.756907565600	T T T
-1.521324591694	3.967075839244	8.618075143800	T T T
-2.869003927994	6.320301933144	8.611769489700	T T T
-5.588091547094	6.313233314144	8.608282602500	T T T
-8.291584485294	11.030529043344	12.902103536300	T T T
-5.574300229894	11.032916671544	12.898781879500	T T T
-4.213334590294	8.676997170044	12.892684777200	T T T
-6.945166319994	11.801659911644	10.751944326600	T T T
-4.222444354394	10.249821826844	10.756907565600	T T T
-4.237964591694	8.672425839244	8.618075143800	T T T
-5.585643927994	11.025651933144	8.611769489700	T T T
-8.304731547094	11.018583314144	8.608282602500	T T T
-11.008224485294	15.735879043344	12.902103536300	T T T
-8.290940229894	15.738266671544	12.898781879500	T T T
-6.929974590294	13.382347170044	12.892684777200	T T T
-9.661806319994	16.507009911644	10.751944326600	T T T
-6.939084354394	14.955171826844	10.756907565600	T T T
-6.954604591694	13.377775839244	8.618075143800	T T T
-8.302283927994	15.731001933144	8.611769489700	T T T
-11.021371547094	15.723933314144	8.608282602500	T T T
-0.141674485294	6.325179043344	12.902103536300	T T T
2.575609770106	6.327566671544	12.898781879500	T T T
3.936575409706	3.971647170044	12.892684777200	T T T
1.204743680006	7.096309911644	10.751944326600	T T T
3.927465645606	5.544471826844	10.756907565600	T T T
3.911945408306	3.967075839244	8.618075143800	T T T
2.564266072006	6.320301933144	8.611769489700	T T T
-0.154821547094	6.313233314144	8.608282602500	T T T
-2.858314485294	11.030529043344	12.902103536300	T T T
-0.141030229894	11.032916671544	12.898781879500	T T T
1.219935409706	8.676997170044	12.892684777200	T T T
-1.511896319994	11.801659911644	10.751944326600	T T T
1.210825645606	10.249821826844	10.756907565600	T T T
1.195305408306	8.672425839244	8.618075143800	T T T
-0.152373927994	11.025651933144	8.611769489700	T T T
-2.871461547094	11.018583314144	8.608282602500	T T T
-5.574954485294	15.735879043344	12.902103536300	T T T
-2.857670229894	15.738266671544	12.898781879500	T T T
-1.496704590294	13.382347170044	12.892684777200	T T T
-4.228536319994	16.507009911644	10.751944326600	T T T
-1.505814354394	14.955171826844	10.756907565600	T T T
-1.521334591694	13.377775839244	8.618075143800	T T T
-2.869013927994	15.731001933144	8.611769489700	T T T
-5.588101547094	15.723933314144	8.608282602500	T T T
5.291595514706	6.325179043344	12.902103536300	T T T
8.008879770106	6.327566671544	12.898781879500	T T T
9.369845409706	3.971647170044	12.892684777200	T T T
6.638013680006	7.096309911644	10.751944326600	T T T
9.360735645606	5.544471826844	10.756907565600	T T T
9.345215408306	3.967075839244	8.618075143800	T T T

7.997536072006	6.320301933144	8.611769489700	T T T
5.278448452906	6.313233314144	8.608282602500	T T T
2.574955514706	11.030529043344	12.902103536300	T T T
5.292239770106	11.032916671544	12.898781879500	T T T
6.653205409706	8.676997170044	12.892684777200	T T T
3.921373680006	11.801659911644	10.751944326600	T T T
6.644095645606	10.249821826844	10.756907565600	T T T
6.628575408306	8.672425839244	8.618075143800	T T T
5.280896072006	11.025651933144	8.611769489700	T T T
2.561808452906	11.018583314144	8.608282602500	T T T
-0.141684485294	15.735879043344	12.902103536300	T T T
2.575599770106	15.738266671544	12.898781879500	T T T
3.936565409706	13.382347170044	12.892684777200	T T T
1.204733680006	16.507009911644	10.751944326600	T T T
3.927455645606	14.955171826844	10.756907565600	T T T
3.911935408306	13.377775839244	8.618075143800	T T T
2.564256072006	15.731001933144	8.611769489700	T T T
-0.154831547094	15.723933314144	8.608282602500	T T T
1.354952130200	0.782228977300	6.382246535200	F F F
-1.361687869800	5.487578977300	6.382246535200	F F F
-4.078327869800	10.192928977300	6.382246535200	F F F
6.788222130200	0.782228977300	6.382246535200	F F F
4.071582130200	5.487578977300	6.382246535200	F F F
1.354942130200	10.192928977300	6.382246535200	F F F
12.221492130200	0.782228977300	6.382246535200	F F F
9.504852130200	5.487578977300	6.382246535200	F F F
6.788212130200	10.192928977300	6.382246535200	F F F

11.3. The 3O-(2x2) Ru(0001) Substrate

commentline Fig. 6 – 3rd point (0.03 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

0.000000000 0.000000000 24.000000000

Ru Si O Os

108 36 72 27

Selective

Cartesian

1.358300000000	2.352700000000	1.000000000000	F	F	F
-1.358300000000	2.352700000000	1.000000000000	F	F	F
2.716600000000	0.000000000000	1.000000000000	F	F	F
0.000000000000	0.000000000000	1.000000000000	F	F	F
1.358300000000	0.784200000000	3.141100000000	F	F	F
4.075000000000	0.784200000000	3.141100000000	F	F	F
0.000000000000	3.136900000000	3.141100000000	F	F	F
2.716600000000	3.136900000000	3.141100000000	F	F	F
1.358313503400	2.351162108900	5.280026634600	T	T	T
4.075377147600	2.322874015600	5.253305043100	T	T	T
2.742248754900	0.023286849500	5.259853613400	T	T	T
5.406265581500	0.022723759800	5.259532133900	T	T	T
-1.358340000000	7.058050000000	1.000000000000	F	F	F
-4.074940000000	7.058050000000	1.000000000000	F	F	F
-0.000040000000	4.705350000000	1.000000000000	F	F	F
-2.716640000000	4.705350000000	1.000000000000	F	F	F
-1.358340000000	5.489550000000	3.141100000000	F	F	F
1.358360000000	5.489550000000	3.141100000000	F	F	F
-2.716640000000	7.842250000000	3.141100000000	F	F	F
-0.000040000000	7.842250000000	3.141100000000	F	F	F
-1.358326496600	7.056512108900	5.280026634600	T	T	T
1.358737147600	7.028224015600	5.253305043100	T	T	T
0.025608754900	4.728636849500	5.259853613400	T	T	T
2.689625581500	4.728073759800	5.259532133900	T	T	T
-4.074980000000	11.763400000000	1.000000000000	F	F	F
-6.791580000000	11.763400000000	1.000000000000	F	F	F
-2.716680000000	9.410700000000	1.000000000000	F	F	F
-5.433280000000	9.410700000000	1.000000000000	F	F	F
-4.074980000000	10.194900000000	3.141100000000	F	F	F
-1.358280000000	10.194900000000	3.141100000000	F	F	F
-5.433280000000	12.547600000000	3.141100000000	F	F	F
-2.716680000000	12.547600000000	3.141100000000	F	F	F
-4.074966496600	11.761862108900	5.280026634600	T	T	T
-1.357902852400	11.733574015600	5.253305043100	T	T	T
-2.691031245100	9.433986849500	5.259853613400	T	T	T
-0.027014418500	9.433423759800	5.259532133900	T	T	T
6.791570000000	2.352700000000	1.000000000000	F	F	F
4.074970000000	2.352700000000	1.000000000000	F	F	F
8.149870000000	0.000000000000	1.000000000000	F	F	F
5.433270000000	0.000000000000	1.000000000000	F	F	F
6.791570000000	0.784200000000	3.141100000000	F	F	F
9.508270000000	0.784200000000	3.141100000000	F	F	F
5.433270000000	3.136900000000	3.141100000000	F	F	F
8.149870000000	3.136900000000	3.141100000000	F	F	F
6.791583503400	2.351162108900	5.280026634600	T	T	T

9.508647147600	2.322874015600	5.253305043100	T T T
8.175518754900	0.023286849500	5.259853613400	T T T
10.839535581500	0.022723759800	5.259532133900	T T T
4.074930000000	7.058050000000	1.000000000000	F F F
1.358330000000	7.058050000000	1.000000000000	F F F
5.433230000000	4.705350000000	1.000000000000	F F F
2.716630000000	4.705350000000	1.000000000000	F F F
4.074930000000	5.489550000000	3.141100000000	F F F
6.791630000000	5.489550000000	3.141100000000	F F F
2.716630000000	7.842250000000	3.141100000000	F F F
5.433230000000	7.842250000000	3.141100000000	F F F
4.074943503400	7.056512108900	5.280026634600	T T T
6.792007147600	7.028224015600	5.253305043100	T T T
5.458878754900	4.728636849500	5.259853613400	T T T
8.122895581500	4.728073759800	5.259532133900	T T T
1.358290000000	11.763400000000	1.000000000000	F F F
-1.358310000000	11.763400000000	1.000000000000	F F F
2.716590000000	9.410700000000	1.000000000000	F F F
-0.000010000000	9.410700000000	1.000000000000	F F F
1.358290000000	10.194900000000	3.141100000000	F F F
4.074990000000	10.194900000000	3.141100000000	F F F
-0.000010000000	12.547600000000	3.141100000000	F F F
2.716590000000	12.547600000000	3.141100000000	F F F
1.358303503400	11.761862108900	5.280026634600	T T T
4.075367147600	11.733574015600	5.253305043100	T T T
2.742238754900	9.433986849500	5.259853613400	T T T
5.406255581500	9.433423759800	5.259532133900	T T T
12.224840000000	2.352700000000	1.000000000000	F F F
9.508240000000	2.352700000000	1.000000000000	F F F
13.583140000000	0.000000000000	1.000000000000	F F F
10.866540000000	0.000000000000	1.000000000000	F F F
12.224840000000	0.784200000000	3.141100000000	F F F
14.941540000000	0.784200000000	3.141100000000	F F F
10.866540000000	3.136900000000	3.141100000000	F F F
13.583140000000	3.136900000000	3.141100000000	F F F
12.224853503400	2.351162108900	5.280026634600	T T T
14.941917147600	2.322874015600	5.253305043100	T T T
13.608788754900	0.023286849500	5.259853613400	T T T
16.272805581500	0.022723759800	5.259532133900	T T T
9.508200000000	7.058050000000	1.000000000000	F F F
6.791600000000	7.058050000000	1.000000000000	F F F
10.866500000000	4.705350000000	1.000000000000	F F F
8.149900000000	4.705350000000	1.000000000000	F F F
9.508200000000	5.489550000000	3.141100000000	F F F
12.224900000000	5.489550000000	3.141100000000	F F F
8.149900000000	7.842250000000	3.141100000000	F F F
10.866500000000	7.842250000000	3.141100000000	F F F
9.508213503400	7.056512108900	5.280026634600	T T T
12.225277147600	7.028224015600	5.253305043100	T T T
10.892148754900	4.728636849500	5.259853613400	T T T
13.556165581500	4.728073759800	5.259532133900	T T T
6.791560000000	11.763400000000	1.000000000000	F F F
4.074960000000	11.763400000000	1.000000000000	F F F
8.149860000000	9.410700000000	1.000000000000	F F F
5.433260000000	9.410700000000	1.000000000000	F F F
6.791560000000	10.194900000000	3.141100000000	F F F
9.508260000000	10.194900000000	3.141100000000	F F F
5.433260000000	12.547600000000	3.141100000000	F F F

8.149860000000	12.547600000000	3.141100000000	F F F
6.791573503400	11.761862108900	5.280026634600	T T T
9.508637147600	11.733574015600	5.253305043100	T T T
8.175508754900	9.433986849500	5.259853613400	T T T
10.839525581500	9.433423759800	5.259532133900	T T T
0.774303866013	4.856953528981	13.007107031100	T T T
3.490891152913	3.273689894681	13.007430676100	T T T
0.774581734513	4.856051215981	9.760138130500	T T T
3.491214311313	3.271378536781	9.760687686500	T T T
-1.942336133987	9.562303528981	13.007107031100	T T T
0.774251152913	7.979039894681	13.007430676100	T T T
-1.942058265487	9.561401215981	9.760138130500	T T T
0.774574311313	7.976728536781	9.760687686500	T T T
-4.658976133987	14.267653528981	13.007107031100	T T T
-1.942388847087	12.684389894681	13.007430676100	T T T
-4.658698265487	14.266751215981	9.760138130500	T T T
-1.942065688687	12.682078536781	9.760687686500	T T T
6.207573866013	4.856953528981	13.007107031100	T T T
8.924161152913	3.273689894681	13.007430676100	T T T
6.207851734513	4.856051215981	9.760138130500	T T T
8.924484311313	3.271378536781	9.760687686500	T T T
3.490933866013	9.562303528981	13.007107031100	T T T
6.207521152913	7.979039894681	13.007430676100	T T T
3.491211734513	9.561401215981	9.760138130500	T T T
6.207844311313	7.976728536781	9.760687686500	T T T
0.774293866013	14.267653528981	13.007107031100	T T T
3.490881152913	12.684389894681	13.007430676100	T T T
0.774571734513	14.266751215981	9.760138130500	T T T
3.491204311313	12.682078536781	9.760687686500	T T T
11.640843866013	4.856953528981	13.007107031100	T T T
14.357431152913	3.273689894681	13.007430676100	T T T
11.641121734513	4.856051215981	9.760138130500	T T T
14.357754311313	3.271378536781	9.760687686500	T T T
8.924203866013	9.562303528981	13.007107031100	T T T
11.640791152913	7.979039894681	13.007430676100	T T T
8.924481734513	9.561401215981	9.760138130500	T T T
11.641114311313	7.976728536781	9.760687686500	T T T
6.207563866013	14.267653528981	13.007107031100	T T T
8.924151152913	12.684389894681	13.007430676100	T T T
6.207841734513	14.266751215981	9.760138130500	T T T
8.924474311313	12.682078536781	9.760687686500	T T T
-0.584252902487	4.065637368881	13.516240097500	T T T
2.132743026113	4.065595371281	13.516402739800	T T T
3.490961451413	1.712544176781	13.550788864800	T T T
0.774709303113	4.891427068181	11.385413272600	T T T
3.491175553613	3.238366226781	11.385882498900	T T T
3.490988261913	1.711138315281	9.209277190200	T T T
2.132459806413	4.062878913981	9.272567338800	T T T
-0.583168357687	4.062588036481	9.272710548300	T T T
-3.300892902487	8.770987368881	13.516240097500	T T T
-0.583896973887	8.770945371281	13.516402739800	T T T
0.774321451413	6.417894176781	13.550788864800	T T T
-1.941930696887	9.596777068181	11.385413272600	T T T
0.774535553613	7.943716226781	11.385882498900	T T T
0.774348261913	6.416488315281	9.209277190200	T T T
-0.584180193587	8.768228913981	9.272567338800	T T T
-3.299808357687	8.767938036481	9.272710548300	T T T
-6.017532902487	13.476337368881	13.516240097500	T T T

-3.300536973887	13.476295371281	13.516402739800	T T T
-1.942318548587	11.123244176781	13.550788864800	T T T
-4.658570696887	14.302127068181	11.385413272600	T T T
-1.942104446387	12.649066226781	11.385882498900	T T T
-1.942291738087	11.121838315281	9.209277190200	T T T
-3.300820193587	13.473578913981	9.272567338800	T T T
-6.016448357687	13.473288036481	9.272710548300	T T T
4.849017097513	4.065637368881	13.516240097500	T T T
7.566013026113	4.065595371281	13.516402739800	T T T
8.924231451413	1.712544176781	13.550788864800	T T T
6.207979303113	4.891427068181	11.385413272600	T T T
8.924445553613	3.238366226781	11.385882498900	T T T
8.924258261913	1.711138315281	9.209277190200	T T T
7.565729806413	4.062878913981	9.272567338800	T T T
4.850101642313	4.062588036481	9.272710548300	T T T
2.132377097513	8.770987368881	13.516240097500	T T T
4.849373026113	8.770945371281	13.516402739800	T T T
6.207591451413	6.417894176781	13.550788864800	T T T
3.491339303113	9.596777068181	11.385413272600	T T T
6.207805553613	7.943716226781	11.385882498900	T T T
6.207618261913	6.416488315281	9.209277190200	T T T
4.849089806413	8.768228913981	9.272567338800	T T T
2.133461642313	8.767938036481	9.272710548300	T T T
-0.584262902487	13.476337368881	13.516240097500	T T T
2.132733026113	13.476295371281	13.516402739800	T T T
3.490951451413	11.123244176781	13.550788864800	T T T
0.774699303113	14.302127068181	11.385413272600	T T T
3.491165553613	12.649066226781	11.385882498900	T T T
3.490978261913	11.121838315281	9.209277190200	T T T
2.132449806413	13.473578913981	9.272567338800	T T T
-0.583178357687	13.473288036481	9.272710548300	T T T
10.282287097513	4.065637368881	13.516240097500	T T T
12.999283026113	4.065595371281	13.516402739800	T T T
14.357501451413	1.712544176781	13.550788864800	T T T
11.641249303113	4.891427068181	11.385413272600	T T T
14.357715553613	3.238366226781	11.385882498900	T T T
14.357528261913	1.711138315281	9.209277190200	T T T
12.99899806413	4.062878913981	9.272567338800	T T T
10.283371642313	4.062588036481	9.272710548300	T T T
7.565647097513	8.770987368881	13.516240097500	T T T
10.282643026113	8.770945371281	13.516402739800	T T T
11.640861451413	6.417894176781	13.550788864800	T T T
8.924609303113	9.596777068181	11.385413272600	T T T
11.641075553613	7.943716226781	11.385882498900	T T T
11.640888261913	6.416488315281	9.209277190200	T T T
10.282359806413	8.768228913981	9.272567338800	T T T
7.566731642313	8.767938036481	9.272710548300	T T T
4.849007097513	13.476337368881	13.516240097500	T T T
7.566003026113	13.476295371281	13.516402739800	T T T
8.924221451413	11.123244176781	13.550788864800	T T T
6.207969303113	14.302127068181	11.385413272600	T T T
8.924435553613	12.649066226781	11.385882498900	T T T
8.924248261913	11.121838315281	9.209277190200	T T T
7.565719806413	13.473578913981	9.272567338800	T T T
4.850091642313	13.473288036481	9.272710548300	T T T
1.356869525200	0.782022843600	6.489933394300	T T T
-0.004821993500	3.145208204300	6.470254528400	T T T
2.721928559300	3.145029146100	6.470293258700	T T T

-1.359770474800	5.487372843600	6.489933394300	T T T
-2.721461993500	7.850558204300	6.470254528400	T T T
0.005288559300	7.850379146100	6.470293258700	T T T
-4.076410474800	10.192722843600	6.489933394300	T T T
-5.438101993500	12.555908204300	6.470254528400	T T T
-2.711351440700	12.555729146100	6.470293258700	T T T
6.790139525200	0.782022843600	6.489933394300	T T T
5.428448006500	3.145208204300	6.470254528400	T T T
8.155198559300	3.145029146100	6.470293258700	T T T
4.073499525200	5.487372843600	6.489933394300	T T T
2.711808006500	7.850558204300	6.470254528400	T T T
5.438558559300	7.850379146100	6.470293258700	T T T
1.356859525200	10.192722843600	6.489933394300	T T T
-0.004831993500	12.555908204300	6.470254528400	T T T
2.721918559300	12.555729146100	6.470293258700	T T T
12.223409525200	0.782022843600	6.489933394300	T T T
10.861718006500	3.145208204300	6.470254528400	T T T
13.588468559300	3.145029146100	6.470293258700	T T T
9.506769525200	5.487372843600	6.489933394300	T T T
8.145078006500	7.850558204300	6.470254528400	T T T
10.871828559300	7.850379146100	6.470293258700	T T T
6.790129525200	10.192722843600	6.489933394300	T T T
5.428438006500	12.555908204300	6.470254528400	T T T
8.155188559300	12.555729146100	6.470293258700	T T T

commentline Fig. 6 – 6th point (0.70 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

0.000000000 0.000000000 24.000000000

Ru Si O Os

108 36 72 27

Selective

Cartesian

1.358300000000	2.352700000000	1.000000000000	F F F
-1.358300000000	2.352700000000	1.000000000000	F F F
2.716600000000	0.000000000000	1.000000000000	F F F
0.000000000000	0.000000000000	1.000000000000	F F F
1.358300000000	0.784200000000	3.141100000000	F F F
4.075000000000	0.784200000000	3.141100000000	F F F
0.000000000000	3.136900000000	3.141100000000	F F F
2.716600000000	3.136900000000	3.141100000000	F F F
1.358313503400	2.351162108900	5.280026634600	T T T
4.075377147600	2.322874015600	5.253305043100	T T T
2.742248754900	0.023286849500	5.259853613400	T T T
5.406265581500	0.022723759800	5.259532133900	T T T
-1.358340000000	7.058050000000	1.000000000000	F F F
-4.074940000000	7.058050000000	1.000000000000	F F F
-0.000040000000	4.705350000000	1.000000000000	F F F
-2.716640000000	4.705350000000	1.000000000000	F F F
-1.358340000000	5.489550000000	3.141100000000	F F F
1.358360000000	5.489550000000	3.141100000000	F F F
-2.716640000000	7.842250000000	3.141100000000	F F F
-0.000040000000	7.842250000000	3.141100000000	F F F

-1.358326496600	7.056512108900	5.280026634600	T T T
1.358737147600	7.028224015600	5.253305043100	T T T
0.025608754900	4.728636849500	5.259853613400	T T T
2.689625581500	4.728073759800	5.259532133900	T T T
-4.074980000000	11.763400000000	1.000000000000	F F F
-6.791580000000	11.763400000000	1.000000000000	F F F
-2.716680000000	9.410700000000	1.000000000000	F F F
-5.433280000000	9.410700000000	1.000000000000	F F F
-4.074980000000	10.194900000000	3.141100000000	F F F
-1.358280000000	10.194900000000	3.141100000000	F F F
-5.433280000000	12.547600000000	3.141100000000	F F F
-2.716680000000	12.547600000000	3.141100000000	F F F
-4.074966496600	11.761862108900	5.280026634600	T T T
-1.357902852400	11.733574015600	5.253305043100	T T T
-2.691031245100	9.433986849500	5.259853613400	T T T
-0.027014418500	9.433423759800	5.259532133900	T T T
6.791570000000	2.352700000000	1.000000000000	F F F
4.074970000000	2.352700000000	1.000000000000	F F F
8.149870000000	0.000000000000	1.000000000000	F F F
5.433270000000	0.000000000000	1.000000000000	F F F
6.791570000000	0.784200000000	3.141100000000	F F F
9.508270000000	0.784200000000	3.141100000000	F F F
5.433270000000	3.136900000000	3.141100000000	F F F
8.149870000000	3.136900000000	3.141100000000	F F F
6.791583503400	2.351162108900	5.280026634600	T T T
9.508647147600	2.322874015600	5.253305043100	T T T
8.175518754900	0.023286849500	5.259853613400	T T T
10.839535581500	0.022723759800	5.259532133900	T T T
4.074930000000	7.058050000000	1.000000000000	F F F
1.358330000000	7.058050000000	1.000000000000	F F F
5.433230000000	4.705350000000	1.000000000000	F F F
2.716630000000	4.705350000000	1.000000000000	F F F
4.074930000000	5.489550000000	3.141100000000	F F F
6.791630000000	5.489550000000	3.141100000000	F F F
2.716630000000	7.842250000000	3.141100000000	F F F
5.433230000000	7.842250000000	3.141100000000	F F F
4.074943503400	7.056512108900	5.280026634600	T T T
6.792007147600	7.028224015600	5.253305043100	T T T
5.458878754900	4.728636849500	5.259853613400	T T T
8.122895581500	4.728073759800	5.259532133900	T T T
1.358290000000	11.763400000000	1.000000000000	F F F
-1.358310000000	11.763400000000	1.000000000000	F F F
2.716590000000	9.410700000000	1.000000000000	F F F
-0.000010000000	9.410700000000	1.000000000000	F F F
1.358290000000	10.194900000000	3.141100000000	F F F
4.074990000000	10.194900000000	3.141100000000	F F F
-0.000010000000	12.547600000000	3.141100000000	F F F
2.716590000000	12.547600000000	3.141100000000	F F F
1.358303503400	11.761862108900	5.280026634600	T T T
4.075367147600	11.733574015600	5.253305043100	T T T
2.742238754900	9.433986849500	5.259853613400	T T T
5.406255581500	9.433423759800	5.259532133900	T T T
12.224840000000	2.352700000000	1.000000000000	F F F
9.508240000000	2.352700000000	1.000000000000	F F F
13.583140000000	0.000000000000	1.000000000000	F F F
10.866540000000	0.000000000000	1.000000000000	F F F
12.224840000000	0.784200000000	3.141100000000	F F F
14.941540000000	0.784200000000	3.141100000000	F F F

10.866540000000	3.136900000000	3.141100000000	F F F
13.583140000000	3.136900000000	3.141100000000	F F F
12.224853503400	2.351162108900	5.280026634600	T T T
14.941917147600	2.322874015600	5.253305043100	T T T
13.608788754900	0.023286849500	5.259853613400	T T T
16.272805581500	0.022723759800	5.259532133900	T T T
9.508200000000	7.058050000000	1.000000000000	F F F
6.791600000000	7.058050000000	1.000000000000	F F F
10.866500000000	4.705350000000	1.000000000000	F F F
8.149900000000	4.705350000000	1.000000000000	F F F
9.508200000000	5.489550000000	3.141100000000	F F F
12.224900000000	5.489550000000	3.141100000000	F F F
8.149900000000	7.842250000000	3.141100000000	F F F
10.866500000000	7.842250000000	3.141100000000	F F F
9.508213503400	7.056512108900	5.280026634600	T T T
12.225277147600	7.028224015600	5.253305043100	T T T
10.892148754900	4.728636849500	5.259853613400	T T T
13.556165581500	4.728073759800	5.259532133900	T T T
6.791560000000	11.763400000000	1.000000000000	F F F
4.074960000000	11.763400000000	1.000000000000	F F F
8.149860000000	9.410700000000	1.000000000000	F F F
5.433260000000	9.410700000000	1.000000000000	F F F
6.791560000000	10.194900000000	3.141100000000	F F F
9.508260000000	10.194900000000	3.141100000000	F F F
5.433260000000	12.547600000000	3.141100000000	F F F
8.149860000000	12.547600000000	3.141100000000	F F F
6.791573503400	11.761862108900	5.280026634600	T T T
9.508637147600	11.733574015600	5.253305043100	T T T
8.175508754900	9.433986849500	5.259853613400	T T T
10.839525581500	9.433423759800	5.259532133900	T T T
-0.083582496650	6.342853610167	13.007107031100	T T T
2.633004790250	4.759589975867	13.007430676100	T T T
-0.083304628150	6.341951297167	9.760138130500	T T T
2.633327948650	4.757278617967	9.760687686500	T T T
-2.800222496650	11.048203610167	13.007107031100	T T T
-0.083635209750	9.464939975867	13.007430676100	T T T
-2.799944628150	11.047301297167	9.760138130500	T T T
-0.083312051350	9.462628617967	9.760687686500	T T T
-5.516862496650	15.753553610167	13.007107031100	T T T
-2.800275209750	14.170289975867	13.007430676100	T T T
-5.516584628150	15.752651297167	9.760138130500	T T T
-2.799952051350	14.167978617967	9.760687686500	T T T
5.349687503350	6.342853610167	13.007107031100	T T T
8.066274790250	4.759589975867	13.007430676100	T T T
5.349965371850	6.341951297167	9.760138130500	T T T
8.066597948650	4.757278617967	9.760687686500	T T T
2.633047503350	11.048203610167	13.007107031100	T T T
5.349634790250	9.464939975867	13.007430676100	T T T
2.633325371850	11.047301297167	9.760138130500	T T T
5.349957948650	9.462628617967	9.760687686500	T T T
-0.083592496650	15.753553610167	13.007107031100	T T T
2.632994790250	14.170289975867	13.007430676100	T T T
-0.083314628150	15.752651297167	9.760138130500	T T T
2.633317948650	14.167978617967	9.760687686500	T T T
10.782957503350	6.342853610167	13.007107031100	T T T
13.499544790250	4.759589975867	13.007430676100	T T T
10.783235371850	6.341951297167	9.760138130500	T T T
13.499867948650	4.757278617967	9.760687686500	T T T

8.066317503350	11.048203610167	13.007107031100	T T T
10.782904790250	9.464939975867	13.007430676100	T T T
8.066595371850	11.047301297167	9.760138130500	T T T
10.783227948650	9.462628617967	9.760687686500	T T T
5.349677503350	15.753553610167	13.007107031100	T T T
8.066264790250	14.170289975867	13.007430676100	T T T
5.349955371850	15.752651297167	9.760138130500	T T T
8.066587948650	14.167978617967	9.760687686500	T T T
-1.442139265150	5.551537450067	13.516240097500	T T T
1.274856663450	5.551495452467	13.516402739800	T T T
2.633075088750	3.198444257967	13.550788864800	T T T
-0.083177059550	6.377327149367	11.385413272600	T T T
2.633289190950	4.724266307967	11.385882498900	T T T
2.633101899250	3.197038396467	9.209277190200	T T T
1.274573443750	5.548778995167	9.272567338800	T T T
-1.441054720350	5.548488117667	9.272710548300	T T T
-4.158779265150	10.256887450067	13.516240097500	T T T
-1.441783336550	10.256845452467	13.516402739800	T T T
-0.083564911250	7.903794257967	13.550788864800	T T T
-2.799817059550	11.082677149367	11.385413272600	T T T
-0.083350809050	9.429616307967	11.385882498900	T T T
-0.083538100750	7.902388396467	9.209277190200	T T T
-1.442066556250	10.254128995167	9.272567338800	T T T
-4.157694720350	10.253838117667	9.272710548300	T T T
-6.875419265150	14.962237450067	13.516240097500	T T T
-4.158423336550	14.962195452467	13.516402739800	T T T
-2.800204911250	12.609144257967	13.550788864800	T T T
-5.516457059550	15.788027149367	11.385413272600	T T T
-2.79990809050	14.134966307967	11.385882498900	T T T
-2.800178100750	12.607738396467	9.209277190200	T T T
-4.158706556250	14.959478995167	9.272567338800	T T T
-6.874334720350	14.959188117667	9.272710548300	T T T
3.991130734850	5.551537450067	13.516240097500	T T T
6.708126663450	5.551495452467	13.516402739800	T T T
8.066345088750	3.198444257967	13.550788864800	T T T
5.350092940450	6.377327149367	11.385413272600	T T T
8.066559190950	4.724266307967	11.385882498900	T T T
8.066371899250	3.197038396467	9.209277190200	T T T
6.707843443750	5.548778995167	9.272567338800	T T T
3.992215279650	5.548488117667	9.272710548300	T T T
1.274490734850	10.256887450067	13.516240097500	T T T
3.991486663450	10.256845452467	13.516402739800	T T T
5.349705088750	7.903794257967	13.550788864800	T T T
2.633452940450	11.082677149367	11.385413272600	T T T
5.349919190950	9.429616307967	11.385882498900	T T T
5.349731899250	7.902388396467	9.209277190200	T T T
3.991203443750	10.254128995167	9.272567338800	T T T
1.275575279650	10.253838117667	9.272710548300	T T T
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1.274846663450	14.962195452467	13.516402739800	T T T
2.633065088750	12.609144257967	13.550788864800	T T T
-0.083187059550	15.788027149367	11.385413272600	T T T
2.633279190950	14.134966307967	11.385882498900	T T T
2.633091899250	12.607738396467	9.209277190200	T T T
1.274563443750	14.959478995167	9.272567338800	T T T
-1.441064720350	14.959188117667	9.272710548300	T T T
9.424400734850	5.551537450067	13.516240097500	T T T
12.141396663450	5.551495452467	13.516402739800	T T T

13.499615088750	3.198444257967	13.550788864800	T T T
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13.499829190950	4.724266307967	11.385882498900	T T T
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12.141113443750	5.548778995167	9.272567338800	T T T
9.425485279650	5.548488117667	9.272710548300	T T T
6.707760734850	10.256887450067	13.516240097500	T T T
9.424756663450	10.256845452467	13.516402739800	T T T
10.782975088750	7.903794257967	13.550788864800	T T T
8.066722940450	11.082677149367	11.385413272600	T T T
10.783189190950	9.429616307967	11.385882498900	T T T
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6.708845279650	10.253838117667	9.272710548300	T T T
3.991120734850	14.962237450067	13.516240097500	T T T
6.708116663450	14.962195452467	13.516402739800	T T T
8.066335088750	12.609144257967	13.550788864800	T T T
5.350082940450	15.788027149367	11.385413272600	T T T
8.066549190950	14.134966307967	11.385882498900	T T T
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3.992205279650	14.959188117667	9.272710548300	T T T
1.356869525200	0.782022843600	6.489933394300	T T T
-0.004821993500	3.145208204300	6.470254528400	T T T
2.721928559300	3.145029146100	6.470293258700	T T T
-1.359770474800	5.487372843600	6.489933394300	T T T
-2.721461993500	7.850558204300	6.470254528400	T T T
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-4.076410474800	10.192722843600	6.489933394300	T T T
-5.438101993500	12.555908204300	6.470254528400	T T T
-2.711351440700	12.555729146100	6.470293258700	T T T
6.790139525200	0.782022843600	6.489933394300	T T T
5.428448006500	3.145208204300	6.470254528400	T T T
8.155198559300	3.145029146100	6.470293258700	T T T
4.073499525200	5.487372843600	6.489933394300	T T T
2.711808006500	7.850558204300	6.470254528400	T T T
5.438558559300	7.850379146100	6.470293258700	T T T
1.356859525200	10.192722843600	6.489933394300	T T T
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2.721918559300	12.555729146100	6.470293258700	T T T
12.223409525200	0.782022843600	6.489933394300	T T T
10.861718006500	3.145208204300	6.470254528400	T T T
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8.145078006500	7.850558204300	6.470254528400	T T T
10.871828559300	7.850379146100	6.470293258700	T T T
6.790129525200	10.192722843600	6.489933394300	T T T
5.428438006500	12.555908204300	6.470254528400	T T T
8.155188559300	12.555729146100	6.470293258700	T T T

commentline Fig. 6 – 13th point (0.0 eV)

1.0000

16.299810000 0.000000000 0.000000000

-8.149920000 14.116050000 0.000000000

```

0.000000000 0.000000000 24.000000000
Ru Si O Os
108 36 72 27
Selective
Cartesian
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-1.358300000000 2.352700000000 1.000000000000 F F F
2.716600000000 0.000000000000 1.000000000000 F F F
0.000000000000 0.000000000000 1.000000000000 F F F
1.358300000000 0.784200000000 3.141100000000 F F F
4.075000000000 0.784200000000 3.141100000000 F F F
0.000000000000 3.136900000000 3.141100000000 F F F
2.716600000000 3.136900000000 3.141100000000 F F F
1.358313503400 2.351162108900 5.280026634600 T T T
4.075377147600 2.322874015600 5.253305043100 T T T
2.742248754900 0.023286849500 5.259853613400 T T T
5.406265581500 0.022723759800 5.259532133900 T T T
-1.358340000000 7.058050000000 1.000000000000 F F F
-4.074940000000 7.058050000000 1.000000000000 F F F
-0.000040000000 4.705350000000 1.000000000000 F F F
-2.716640000000 4.705350000000 1.000000000000 F F F
-1.358340000000 5.489550000000 3.141100000000 F F F
1.358360000000 5.489550000000 3.141100000000 F F F
-2.716640000000 7.842250000000 3.141100000000 F F F
-0.000040000000 7.842250000000 3.141100000000 F F F
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0.025608754900 4.728636849500 5.259853613400 T T T
2.689625581500 4.728073759800 5.259532133900 T T T
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-6.791580000000 11.763400000000 1.000000000000 F F F
-2.716680000000 9.410700000000 1.000000000000 F F F
-5.433280000000 9.410700000000 1.000000000000 F F F
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-1.358280000000 10.194900000000 3.141100000000 F F F
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-2.691031245100 9.433986849500 5.259853613400 T T T
-0.027014418500 9.433423759800 5.259532133900 T T T
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4.074970000000 2.352700000000 1.000000000000 F F F
8.149870000000 0.000000000000 1.000000000000 F F F
5.433270000000 0.000000000000 1.000000000000 F F F
6.791570000000 0.784200000000 3.141100000000 F F F
9.508270000000 0.784200000000 3.141100000000 F F F
5.433270000000 3.136900000000 3.141100000000 F F F
8.149870000000 3.136900000000 3.141100000000 F F F
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9.508647147600 2.322874015600 5.253305043100 T T T
8.175518754900 0.023286849500 5.259853613400 T T T
10.839535581500 0.022723759800 5.259532133900 T T T
4.074930000000 7.058050000000 1.000000000000 F F F
1.358330000000 7.058050000000 1.000000000000 F F F
5.433230000000 4.705350000000 1.000000000000 F F F
2.716630000000 4.705350000000 1.000000000000 F F F
4.074930000000 5.489550000000 3.141100000000 F F F

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6.791630000000	5.489550000000	3.141100000000	F F F
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5.433230000000	7.842250000000	3.141100000000	F F F
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5.458878754900	4.728636849500	5.259853613400	T T T
8.122895581500	4.728073759800	5.259532133900	T T T
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-1.358310000000	11.763400000000	1.000000000000	F F F
2.716590000000	9.410700000000	1.000000000000	F F F
-0.000010000000	9.410700000000	1.000000000000	F F F
1.358290000000	10.194900000000	3.141100000000	F F F
4.074990000000	10.194900000000	3.141100000000	F F F
-0.000010000000	12.547600000000	3.141100000000	F F F
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9.508240000000	2.352700000000	1.000000000000	F F F
13.583140000000	0.000000000000	1.000000000000	F F F
10.866540000000	0.000000000000	1.000000000000	F F F
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14.941917147600	2.322874015600	5.253305043100	T T T
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8.149860000000	12.547600000000	3.141100000000	F F F
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-2.085039177501	9.809050972423	9.760138130500	T T T

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-7.518597046001	19.220653285423	13.007107031100	T T T
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3.347952953999	9.809953285423	13.007107031100	T T T
6.064540240899	8.226689651123	13.007430676100	T T T
3.348230822499	9.809050972423	9.760138130500	T T T
6.064863399299	8.224378293223	9.760687686500	T T T
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-8.876069269701	18.426287792923	9.272710548300	T T T
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6.064610539399	6.665543933223	13.550788864800	T T T
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6.064637349899	6.664138071723	9.209277190200	T T T
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4.707110730299	13.720937792923	9.272710548300	T T T
1.989386185499	18.429337125323	13.516240097500	T T T
4.706382114099	18.429295127723	13.516402739800	T T T
6.064600539399	16.076243933223	13.550788864800	T T T
3.348348391099	19.255126824623	11.385413272600	T T T
6.064814641599	17.602065983223	11.385882498900	T T T
6.064627349899	16.074838071723	9.209277190200	T T T
4.706098894399	18.426578670423	9.272567338800	T T T
1.990470730299	18.426287792923	9.272710548300	T T T
1.356869525200	0.782022843600	6.489933394300	T T T
-0.004821993500	3.145208204300	6.470254528400	T T T
2.721928559300	3.145029146100	6.470293258700	T T T
-1.359770474800	5.487372843600	6.489933394300	T T T
-2.721461993500	7.850558204300	6.470254528400	T T T
0.005288559300	7.850379146100	6.470293258700	T T T
-4.076410474800	10.192722843600	6.489933394300	T T T
-5.438101993500	12.555908204300	6.470254528400	T T T
-2.711351440700	12.555729146100	6.470293258700	T T T
6.790139525200	0.782022843600	6.489933394300	T T T
5.428448006500	3.145208204300	6.470254528400	T T T

8.155198559300	3.145029146100	6.470293258700	T T T
4.073499525200	5.487372843600	6.489933394300	T T T
2.711808006500	7.850558204300	6.470254528400	T T T
5.438558559300	7.850379146100	6.470293258700	T T T
1.356859525200	10.192722843600	6.489933394300	T T T
-0.004831993500	12.555908204300	6.470254528400	T T T
2.721918559300	12.555729146100	6.470293258700	T T T
12.223409525200	0.782022843600	6.489933394300	T T T
10.861718006500	3.145208204300	6.470254528400	T T T
13.588468559300	3.145029146100	6.470293258700	T T T
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8.145078006500	7.850558204300	6.470254528400	T T T
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6.790129525200	10.192722843600	6.489933394300	T T T
5.428438006500	12.555908204300	6.470254528400	T T T
8.155188559300	12.555729146100	6.470293258700	T T T

commentline Fig. 6 – 20th point (0.51 eV)

1.0

+16.2998100000 +0.0000000000 +0.0000000000
 -8.1499200000 +14.1160500000 +0.0000000000
 +0.0000000000 +0.0000000000 +24.0000000000

Ru Si O Os

108 36 72 27

Selective

Cartesian

+1.3583000000	+2.3527000000	+1.0000000000	F F F
-1.3583000000	+2.3527000000	+1.0000000000	F F F
+2.7166000000	+0.0000000000	+1.0000000000	F F F
+0.0000000000	+0.0000000000	+1.0000000000	F F F
+1.3583000000	+0.7842000000	+3.1411000000	F F F
+4.0750000000	+0.7842000000	+3.1411000000	F F F
-0.0000000000	+3.1369000000	+3.1411000000	F F F
+2.7166000000	+3.1369000000	+3.1411000000	F F F
+1.3583135034	+2.3511621089	+5.2800266346	T T T
+4.0753771476	+2.3228740156	+5.2533050431	T T T
+2.7422487549	+0.0232868495	+5.2598536134	T T T
+5.4062655815	+0.0227237598	+5.2595321339	T T T
-1.3583400000	+7.0580500000	+1.0000000000	F F F
-4.0749400000	+7.0580500000	+1.0000000000	F F F
-0.0000400000	+4.7053500000	+1.0000000000	F F F
-2.7166400000	+4.7053500000	+1.0000000000	F F F
-1.3583400000	+5.4895500000	+3.1411000000	F F F
+1.3583600000	+5.4895500000	+3.1411000000	F F F
-2.7166400000	+7.8422500000	+3.1411000000	F F F
-0.0000400000	+7.8422500000	+3.1411000000	F F F
-1.3583264966	+7.0565121089	+5.2800266346	T T T
+1.3587371476	+7.0282240156	+5.2533050431	T T T
+0.0256087549	+4.7286368495	+5.2598536134	T T T
+2.6896255815	+4.7280737598	+5.2595321339	T T T
-4.0749800000	+11.7634000000	+1.0000000000	F F F
-6.7915800000	+11.7634000000	+1.0000000000	F F F
-2.7166800000	+9.4107000000	+1.0000000000	F F F
-5.4332800000	+9.4107000000	+1.0000000000	F F F

-4.0749800000 +10.1949000000 +3.1411000000 F F F
 -1.3582800000 +10.1949000000 +3.1411000000 F F F
 -5.4332800000 +12.5476000000 +3.1411000000 F F F
 -2.7166800000 +12.5476000000 +3.1411000000 F F F
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 -1.3579028524 +11.7335740156 +5.2533050431 T T T
 -2.6910312451 +9.4339868495 +5.2598536134 T T T
 -0.0270144185 +9.4334237598 +5.2595321339 T T T
 +6.7915700000 +2.3527000000 +1.0000000000 F F F
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