Supporting Information

Tritium Adsorption and Absorption on (100) and (001) Surfaces of Pure and Tin Defective Zirconium

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S1. Default and Modified H POTCAR Energies

In this and previous studies we have modified the mass of hydrogen in the POTCAR file to better represent tritium (T).[1-3] This only affects the lattice dynamics and phonons, items that were not investigated in this study. The differences (or lack thereof) in energy are given below in Table S1, with the computational details given in the main text.

Table S1. Energy comparison for ^{1}H and T systems.

System	H	H_2	H_2O	H on Zr(001) (HCP site)	H on Zr(100) (step site)
Energy with ^{1}H (eV)	-0.9112	-6.8202	-12.2184	-602.2928	-531.6119
Energy with T (eV)	-0.9112	-6.8202	-12.2184	-602.2928	-531.6119

S2. Surface Energy Convergence

To confirm that the Zr slabs used to model the surface were of sufficient layers to perform accurately, the surface energy as a functional of Zr layers was investigated. The surface energy was calculated according to Equation S1, where $E_{Slab}$is the energy of the slab, N is the number of atoms, E_{Bulk} is energy per atom in the bulk, A is the surface area, and γ is the surface energy.

$$\gamma = \frac{E_{Slab} - NE_{Bulk}}{2A} \tag{S1}$$

Zr(001) was built using layers of 25 atoms, with each layer stacking above another in the direction of the *c*-axis. The surface energy was converged to within 0.01 J/m2 after four layers of atoms, which was used as the convergence criteria. The energy per layer for Zr(001) is displayed in Figure S1.

Zr(100) was constructed using layers of 15 atoms, with each layer stacking above another in the direction of the *a*-axis. The Zr(100) surface features two different terminations, a more stable surface occurring when an even number of layers is present, and a less stable surface occurring with an odd number of layers present. For the more stable termination, the surface energy was converged with six layers of atoms. The energy per layer for Zr(100) is displayed in Figure S2.

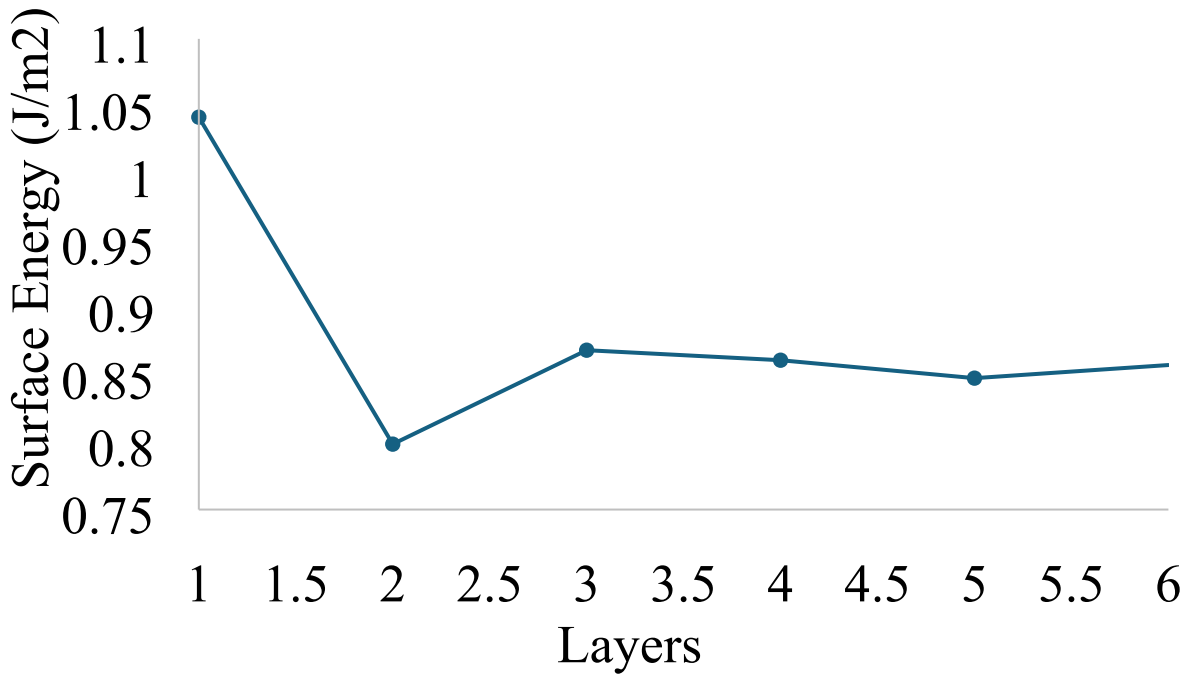

Figure S1. Surface energy as a function of layers of 25 atoms for Zr(001).

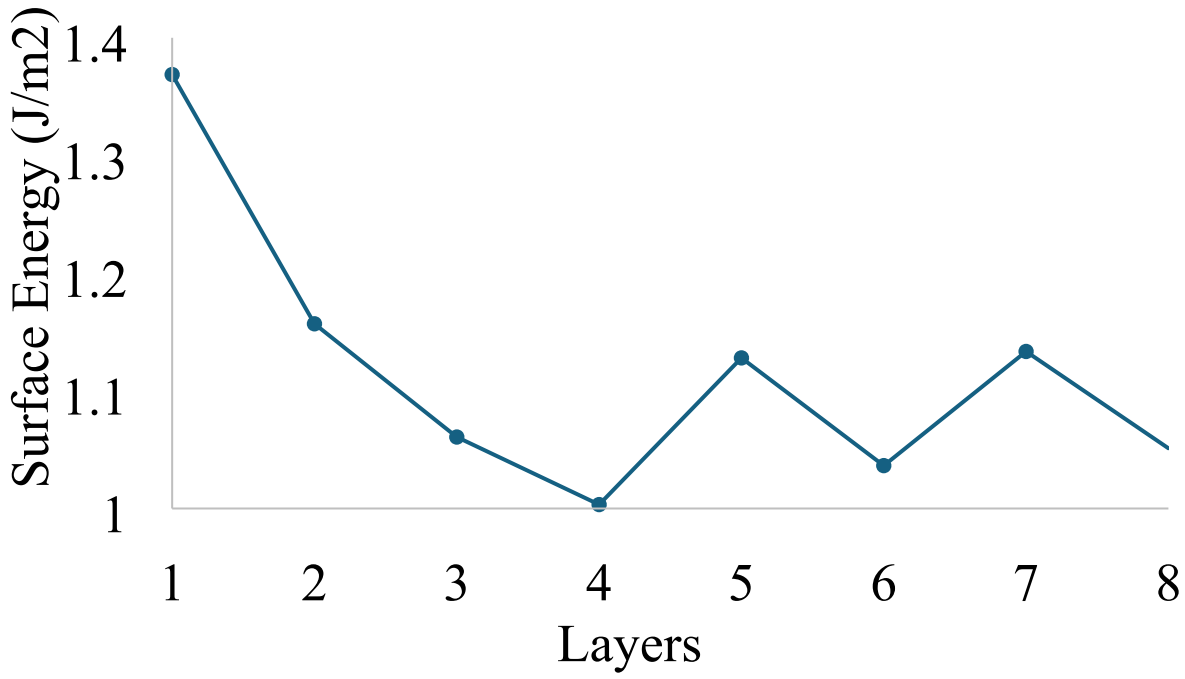

Figure S2. Surface energy as a function of layers of 15 atoms for Zr(100).

S3. Frozen Layers Convergence

For surface studies, it is common to freeze layers of the substrate, starting with those farthest from the surface, in order to reduce computational cost. Layers far from the surface may not participate in surface-adsorbate interactions, however this must be confirmed. The effect of this was investigated by optimizing a T atom on the Zr surfaces with varying amounts of frozen layers. The case where all layers were frozen was neglected for both Zr(001) and Zr(100). For Zr(001), a T atom was placed on an hexagonal close packed (HCP) site and the number of frozen layers was varied from three frozen layers (only the top layer allowed to relax) to zero frozen layers (all layers allowed to relax). For Zr(100), a T atom was placed on a bridge site and the number of frozen layers was varied from five frozen layers (only the top layer allowed to relax) to zero frozen layers (all layers allowed to relax). These convergence tests are displayed visually in Figures S3 and S4.

For all systems, the energy per Zr atom differences as a function of frozen layers are less than a single meV/atom regardless of the number of frozen layers. This minute energy difference is well within the tolerance to which the computational parameters were converged. Allowing half of the layers to freely relax for each system, that being two frozen layers and two free layers for Zr(001) and three frozen layers with three free layers for Zr(100), was selected to reduce computational expense while maintaining accuracy.

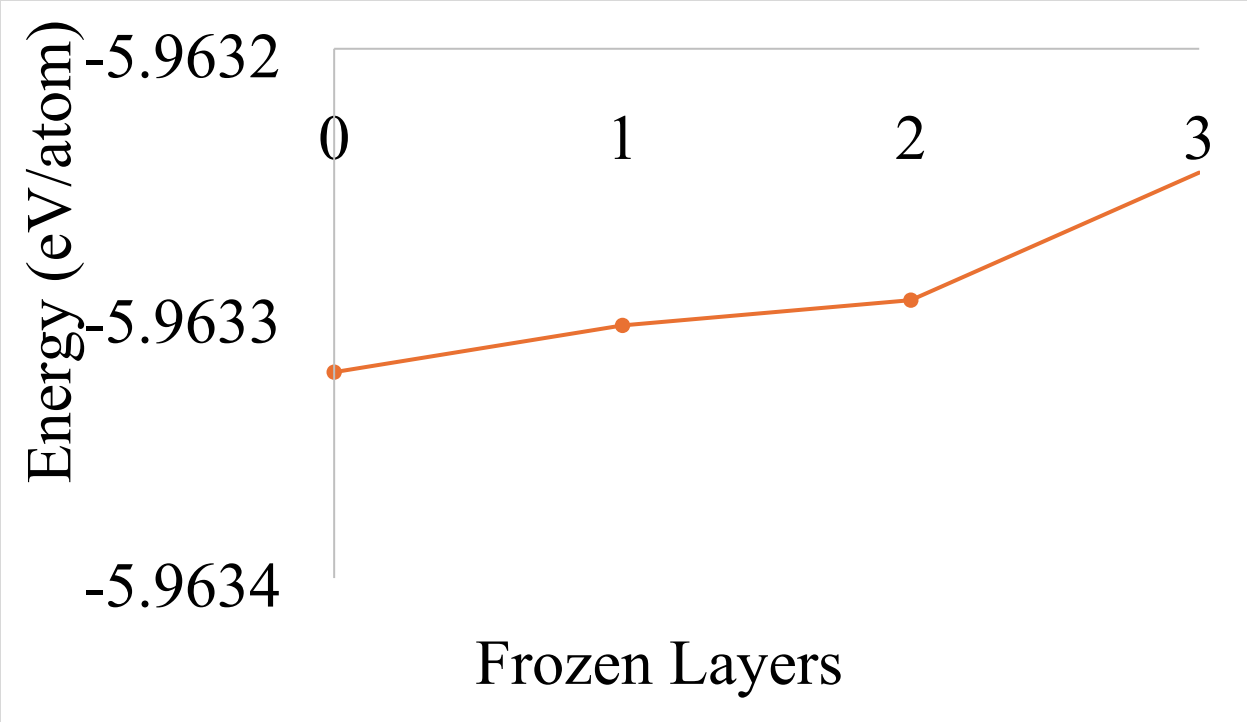

Figure S3. Energy as a function of frozen layers for Zr(001)

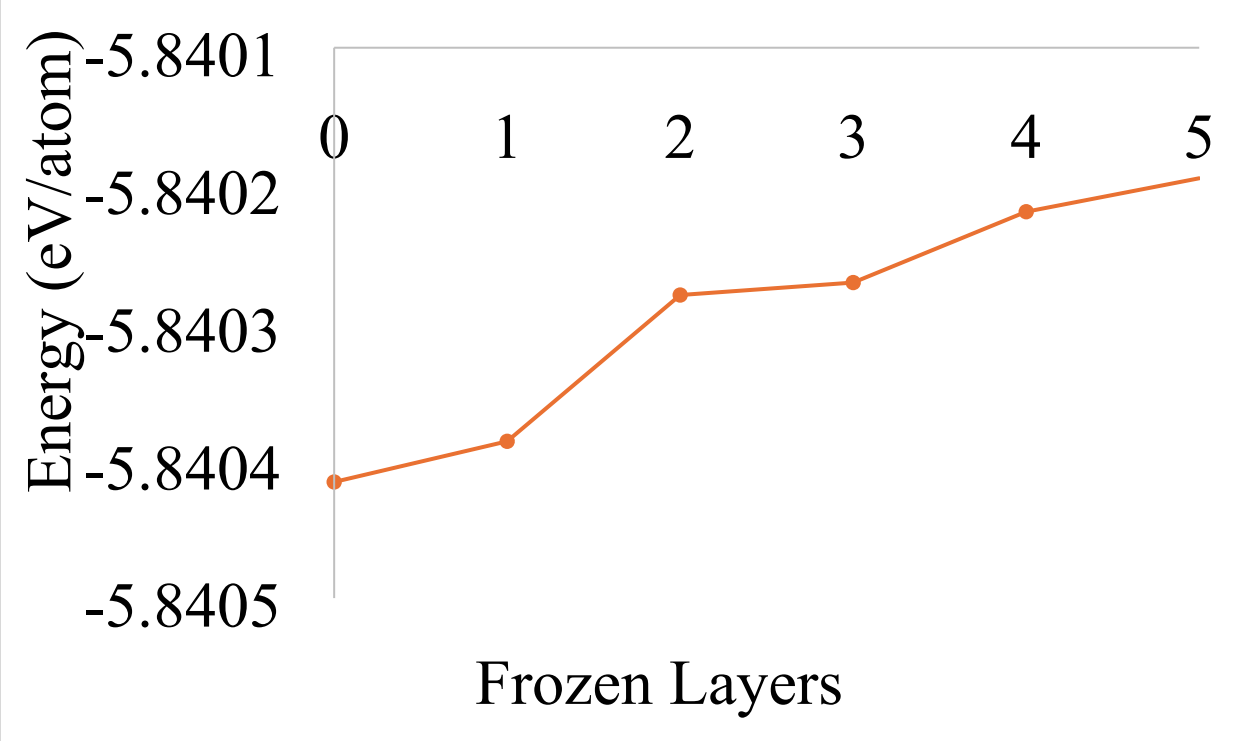

Figure S4. Energy as a function of frozen layers for Zr(100).

S4. Bader Charges

To determine the charge transfer from the Zr surfaces to the adsorbed and absorbed T atoms and T_2 molecules, Bader charges were calculated. A larger charge transfer from the surface of the adsorbent to the adsorbed moiety may be indicative of stronger bonding, resulting in a more stable (more negative) binding energy. Sites with less charge transfer, such as T on a top or bridge site of Zr (001) have less favorable binding energies, however this behavior is not always a one-to-one relation, as seen on the Zr (100) surface.

Table S2. Charge transfer from Zr surfaces to T. A positive value of charge transfer indicates charge transfer from the surface to the T.

Surface	**(001)**	**(001)**	**(001)**	**(001)**	**(100)**	**(100)**	**(100)**
Binding Site	Top	Bridge	HCP	FCC	Upper Bridge	Lower Bridge	Step
Charge Transfer (e^-)	0.52	0.62	0.64	0.64	0.59	0.66	0.63

Table S3. Charge transfer from Zr surfaces to T_2. A single listed site means that dissociation of T_2 was not observed (*), while two listed sites indicate dissociation of T_2 into two separate T atoms (**). Bader charges are omitted where the T_2 dissociated. A positive value of charge transfer indicates charge transfer from the surface to the T. Bader charges for the dissociated T atoms are provided in Table S2.

Surface	**(001)***	**(001)***	**(001)****	**(001)****	**(100)***	**(100)****	**(100)****
Binding Site(s)	Top	FCC	Bridge, HCP	2x HCP	Top	2x Upper Bridge	2x Lower Bridge
Charge Transfer (e^-)	0.31, 0.31	0.16 (closer to Zr), 0.07 (further from Zr)	--	--	--	--	--

Table S4. Charge transfer from Sn defective Zr surfaces to T. A positive value of charge transfer indicates charge transfer from the surface to the T. Bader charges are omitted where the Sn repulsed the T to a different site. Bader charges for T atoms on Zr are provided in Table S2.

Surface	**(001)**	**(001)**	**(001)**	**(001)**	**(100)**	**(100)**	**(100)**
Initial Site	Top	Bridge	HCP	FCC	Upper Bridge	Lower Bridge	Step
Final Site	Top	Bridge	FCC	HCP	Upper Bridge	Step	Lower Bridge
Final Site on Sn?	Yes	Yes	No	No	Yes	No	No
Charge Transfer (e^-)	0.38	0.49	--	--	0.48	--	--

Table S5. Charge transfer from Sn defective Zr surfaces to T_2. A positive value of charge transfer indicates charge transfer from the surface to the T_2. Bader charges are omitted where the Sn repulsed the T_2 to a different site.

Surface	**(001)**	**(001)**	**(001)**	**(001)**	**(001)**	**(100)**	**(100)**	**(100)**
Initial Site	Top	Bridge (T_2 parallel)	Bridge (T_2 perpendicular)	HCP	FCC	Upper Bridge	Lower Bridge	Step
Final Site	Top	Top	HCP FCC	Top	HCP (off Sn) FCC (on Sn)	Top	Upper Bridge Upper Bridge	Lower Bridge
Dissociated?	No	No	Yes	No	Yes	No	Yes	No
Final Site(s) on Sn?	No	No	No	No	FCC	No	No	No
Charge Transfer (e^-)	--	--	--	--	0.60 (off Sn) 0.49 (on Sn)	--	--	--

Table S6. Charge transfer from Zr(001) to T during the absorption process. A positive value of charge transfer indicates charge transfer from the adsorbent to the T.

Site	Surface FCC	Subsurface Octahedral	Bulk Octahedral

Charge Transfer (e^-)	0.64	0.66	0.69

Table S7. Charge transfer from Zr(100) to T during the absorption process. A positive value of charge transfer indicates charge transfer from the adsorbent to the T.

Site	Surface Step	Subsurface Tetrahedral
Charge Transfer (e^-)	0.63	0.66

Table S8. Charge transfer from surface Sn defective Zr(001) to T during the absorption process. A positive value of charge transfer indicates charge transfer from the adsorbent to the T.

Site	Surface FCC, Sn defective	Subsurface Octahedral
Charge Transfer (e^-)	0.63	0.64

Table S9. Charge transfer from subsurface Sn defective Zr(001) to T during the absorption process. A positive value of charge transfer indicates charge transfer from the adsorbent to the T.

Site	Surface FCC	Subsurface Octahedral, Sn defective	Bulk Octahedral, Sn defective
Charge Transfer (e^-)	0.64	0.69	0.67

S5. Density of States

To investigate the interaction between the Zr surfaces and the adsorbed and absorbed T atoms and T_2 molecules, the projected density of states (DOS) of the systems were calculated. A shift in the projected density of states (pDOS) of the isolated moiety compared and surface compared to that of the combined system can be indicative of binding interaction, especially if there is overlap in the adsorbent and moiety states. The overlap in the pDOS and the effect on binding energy can be clearly observed in Figures S5, S8, and S12-15, as an increase in overlap in the pDOS for the binding sites corresponds to a more favorable binding energy.

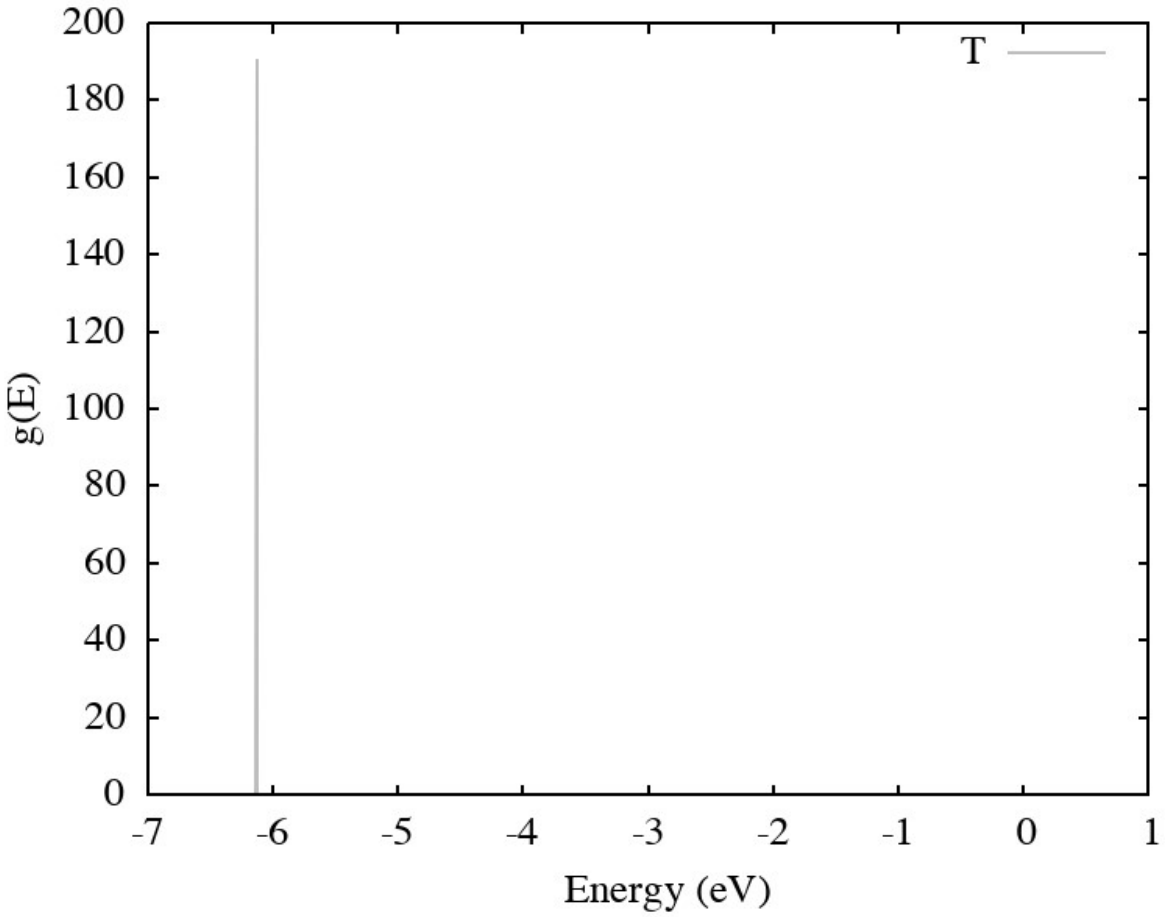

Figure S5. Density of states for T in the gas phase.

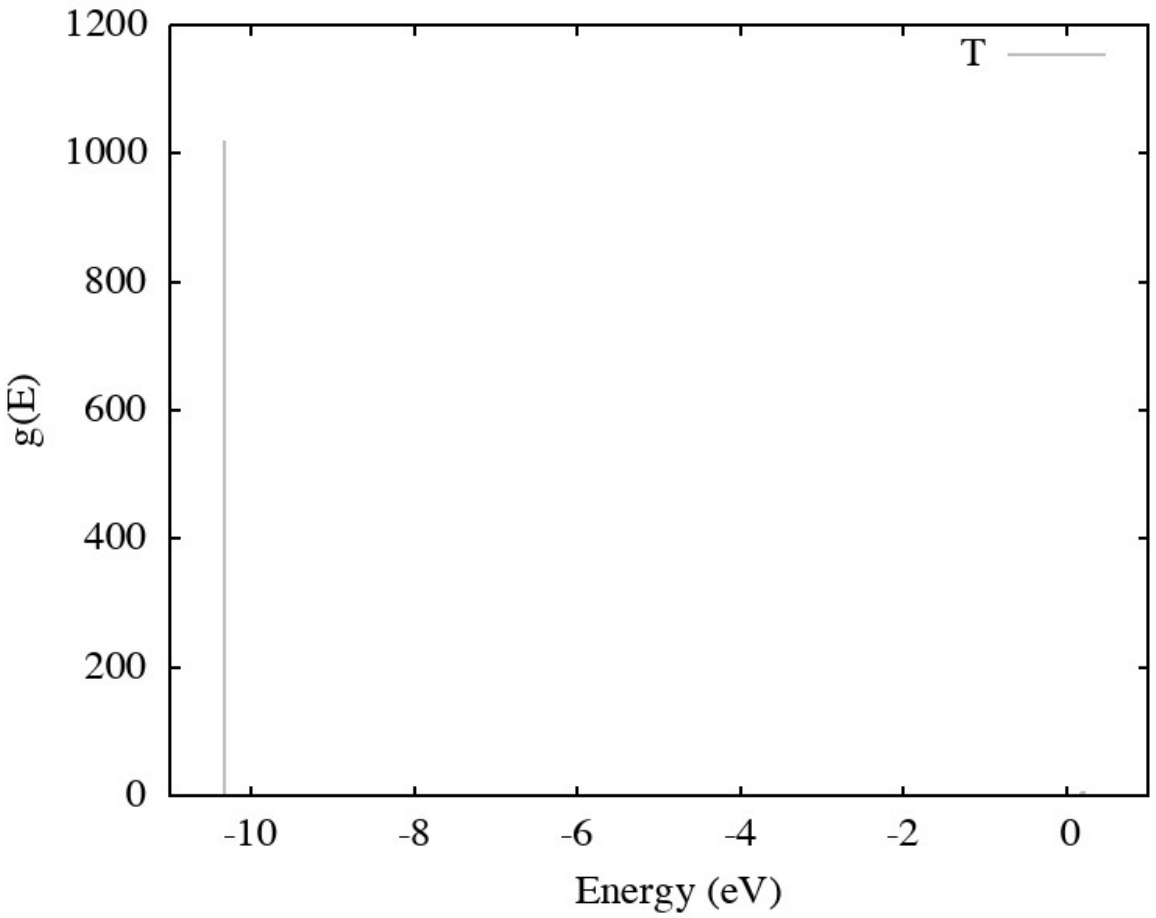

Figure S6. Density of states for T_2 in the gas phase.

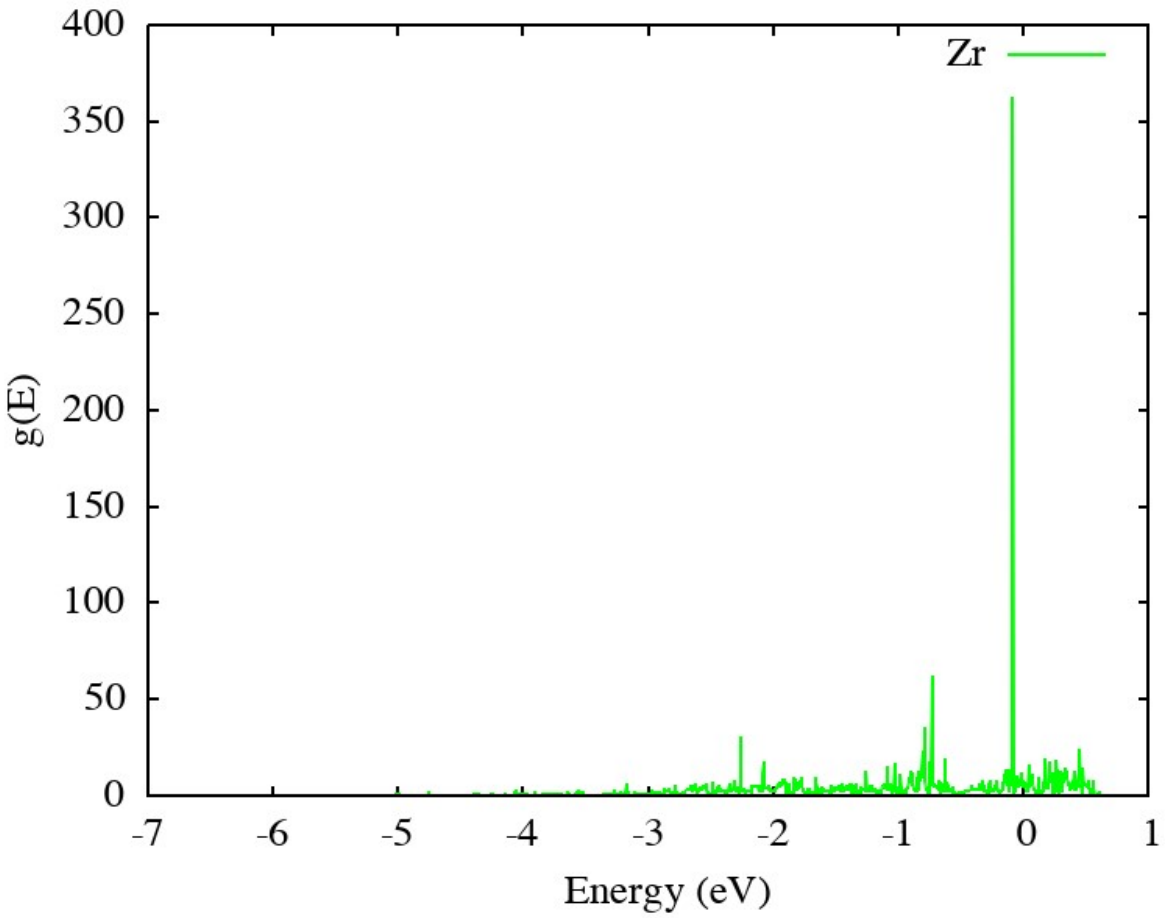

Figure S7. Density of states for Zr(001).

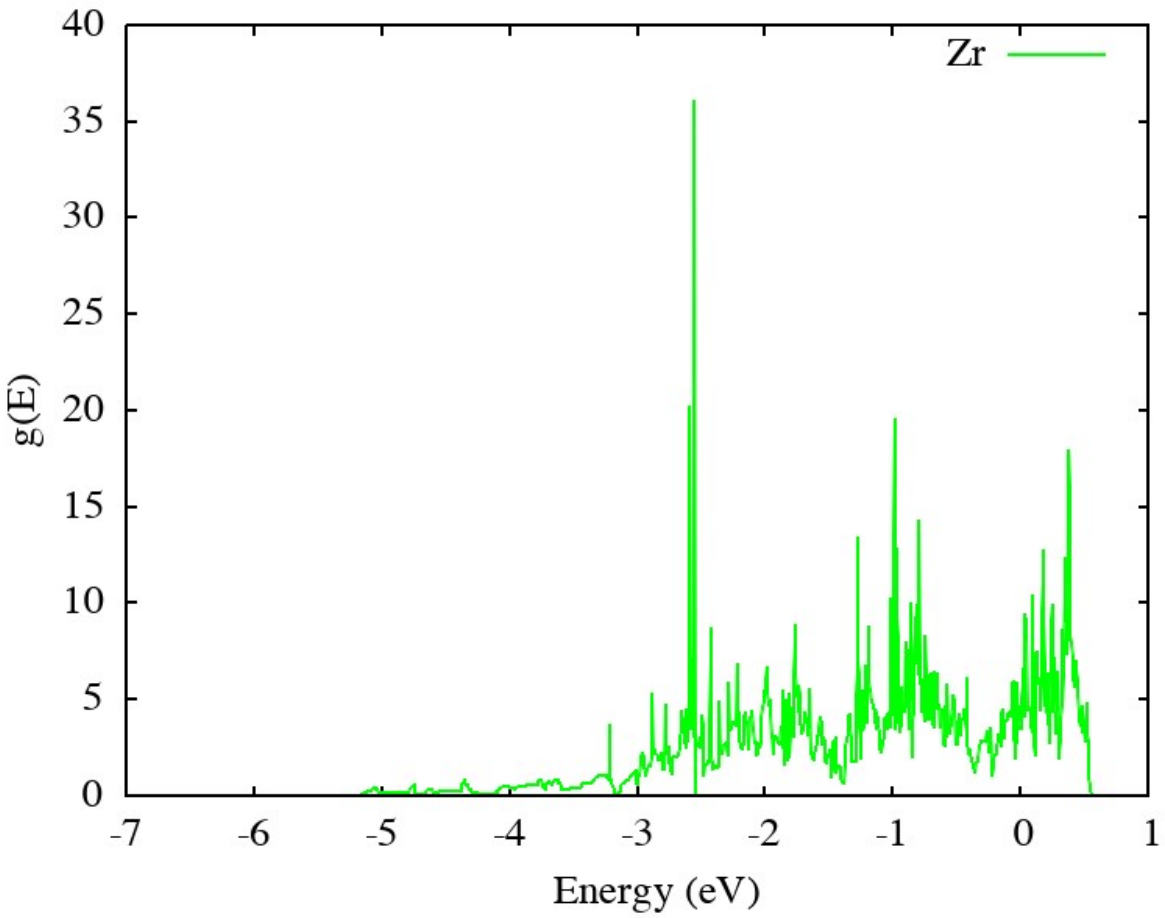

Figure S8. Density of states for Zr(100).

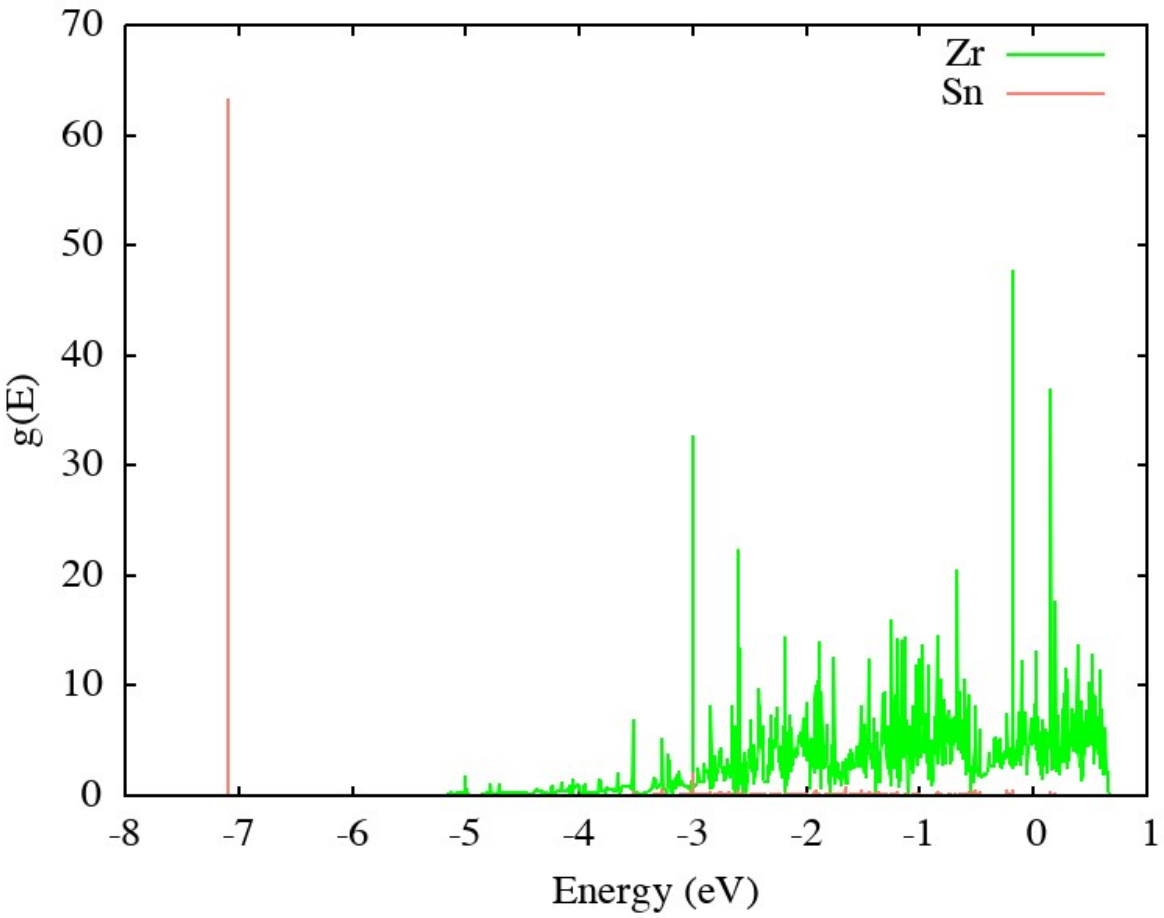

Figure S9. Density of states for Zr(001) with a surface Sn defect.

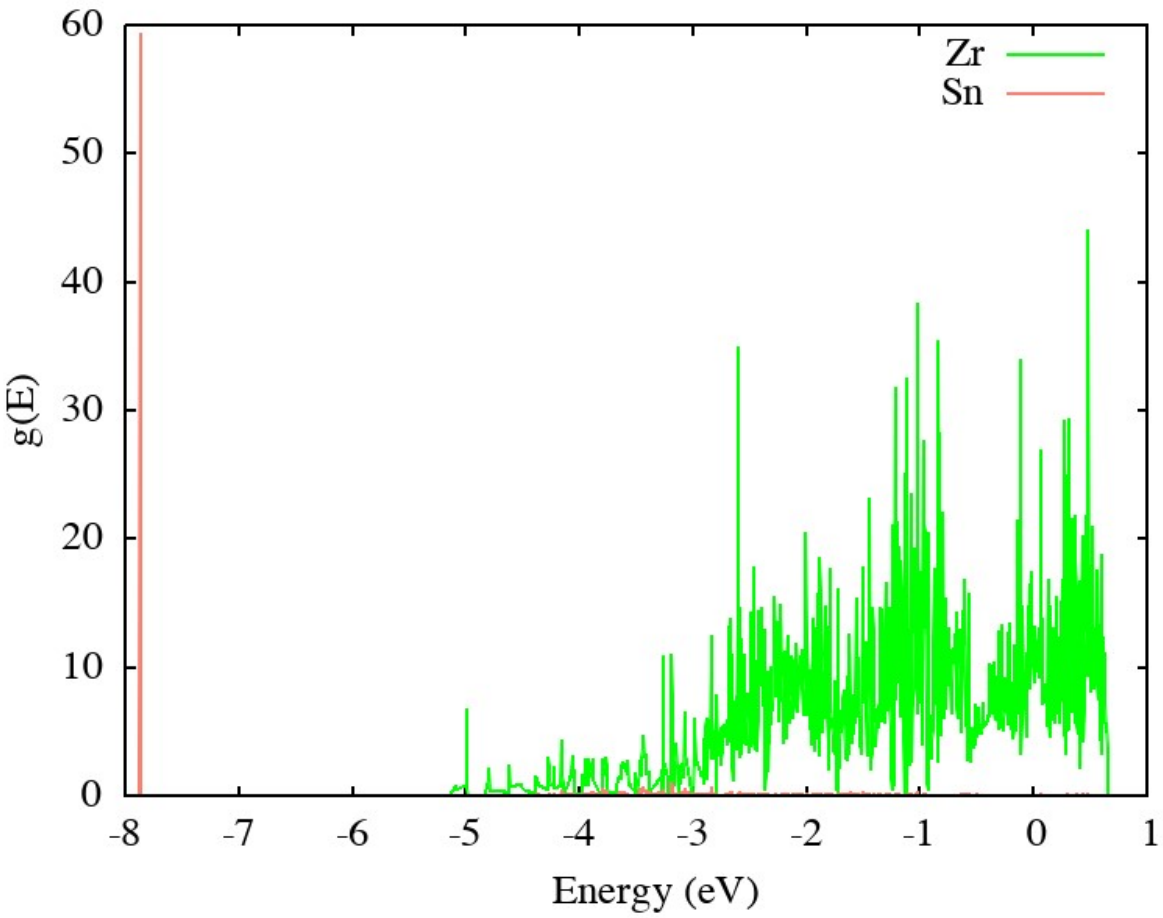

Figure S10. Density of states for Zr(001) with a subsurface Sn defect.

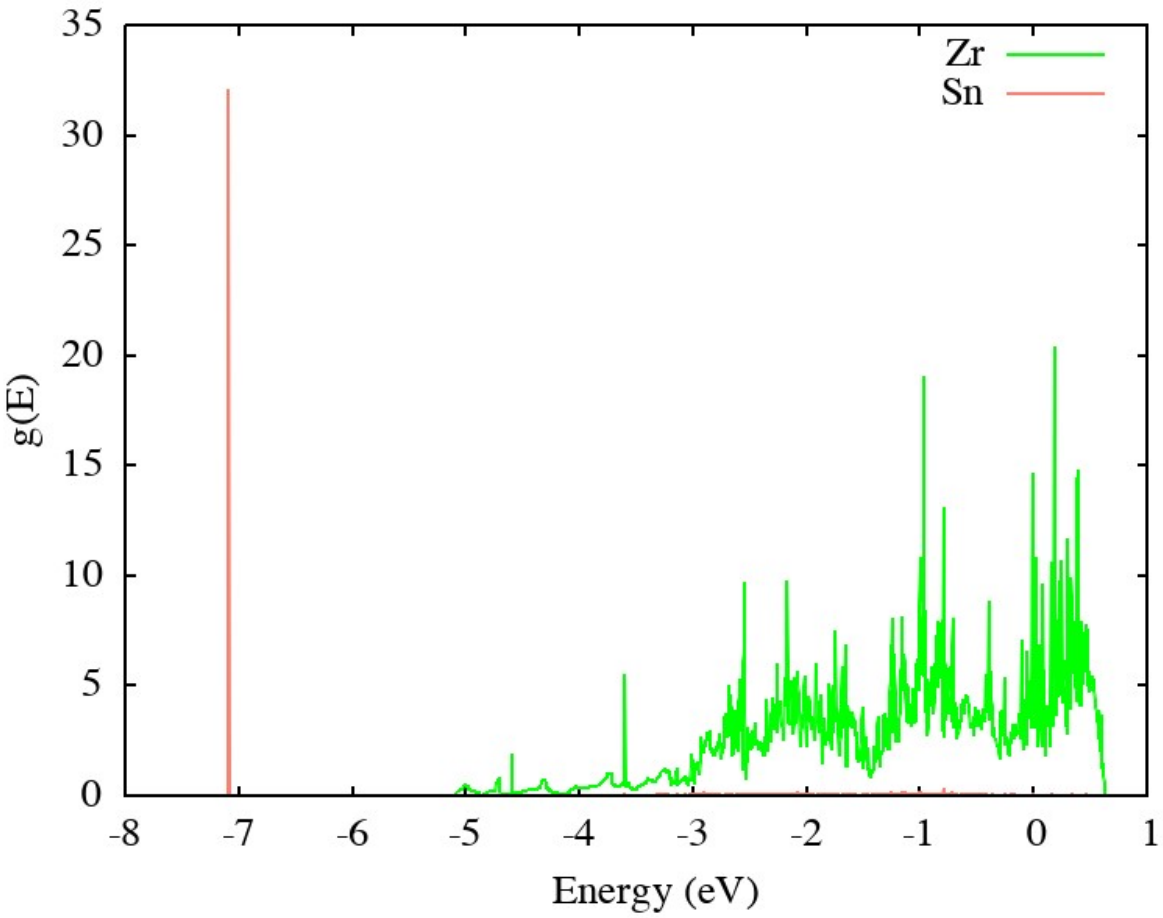

Figure S11. Density of states for Zr(100) with a surface Sn defect.

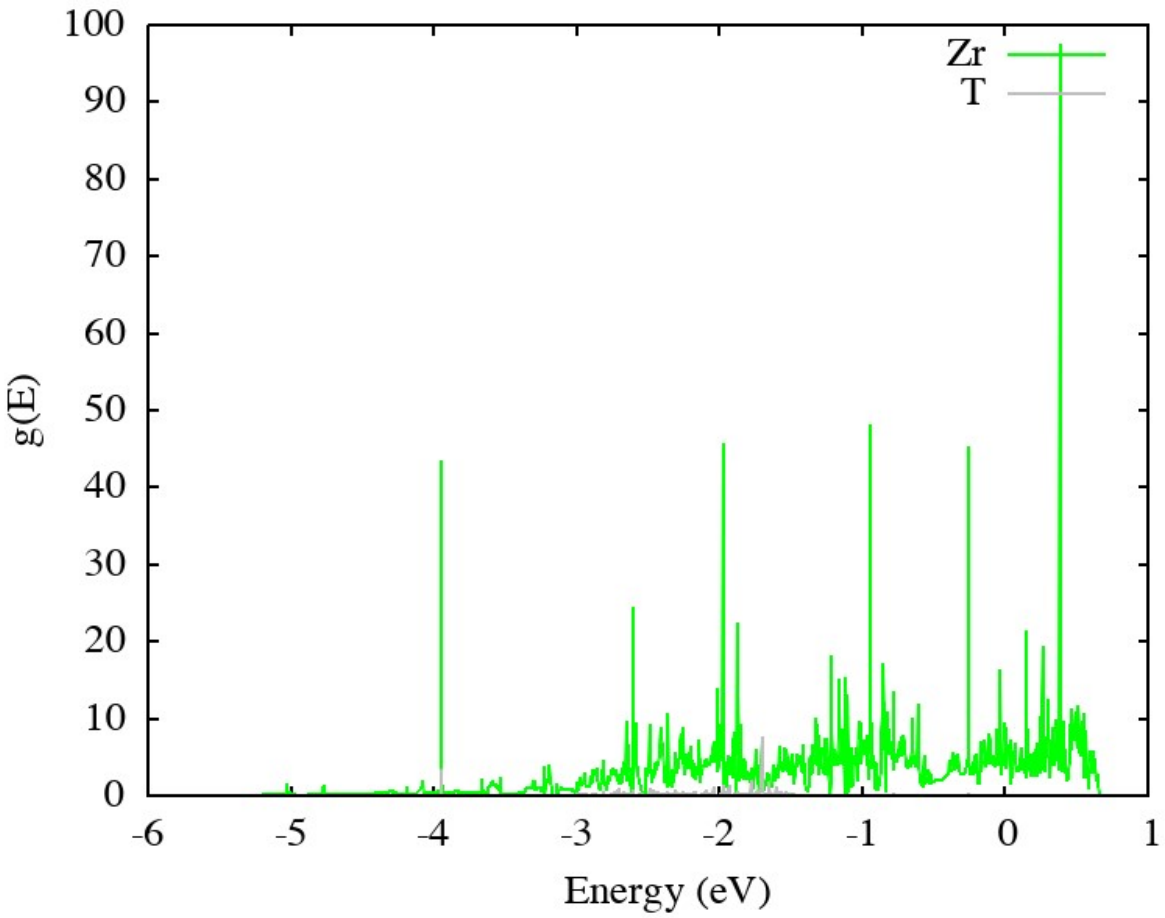

Figure S12. Projected density of states for T on a top site of Zr(001).

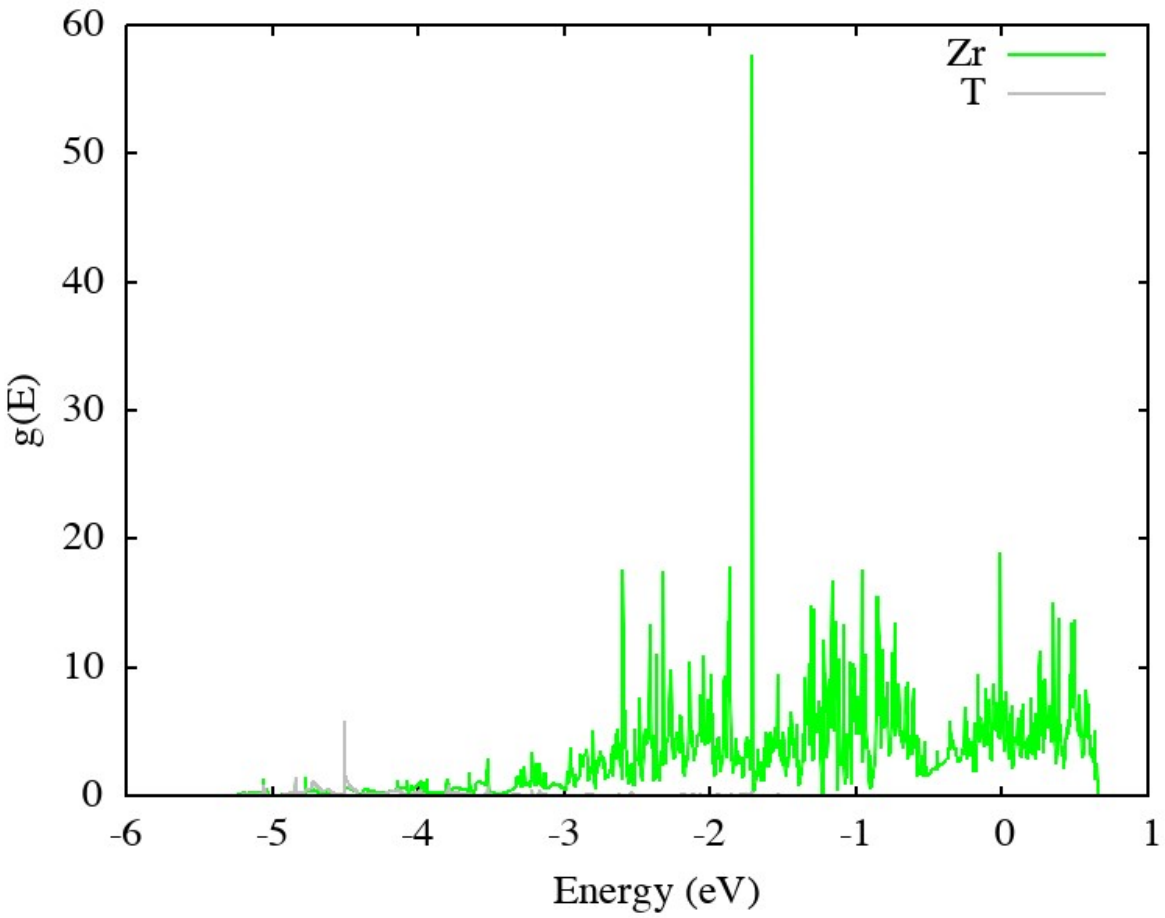

Figure S13. Projected density of states for T on a bridge site of Zr(001).

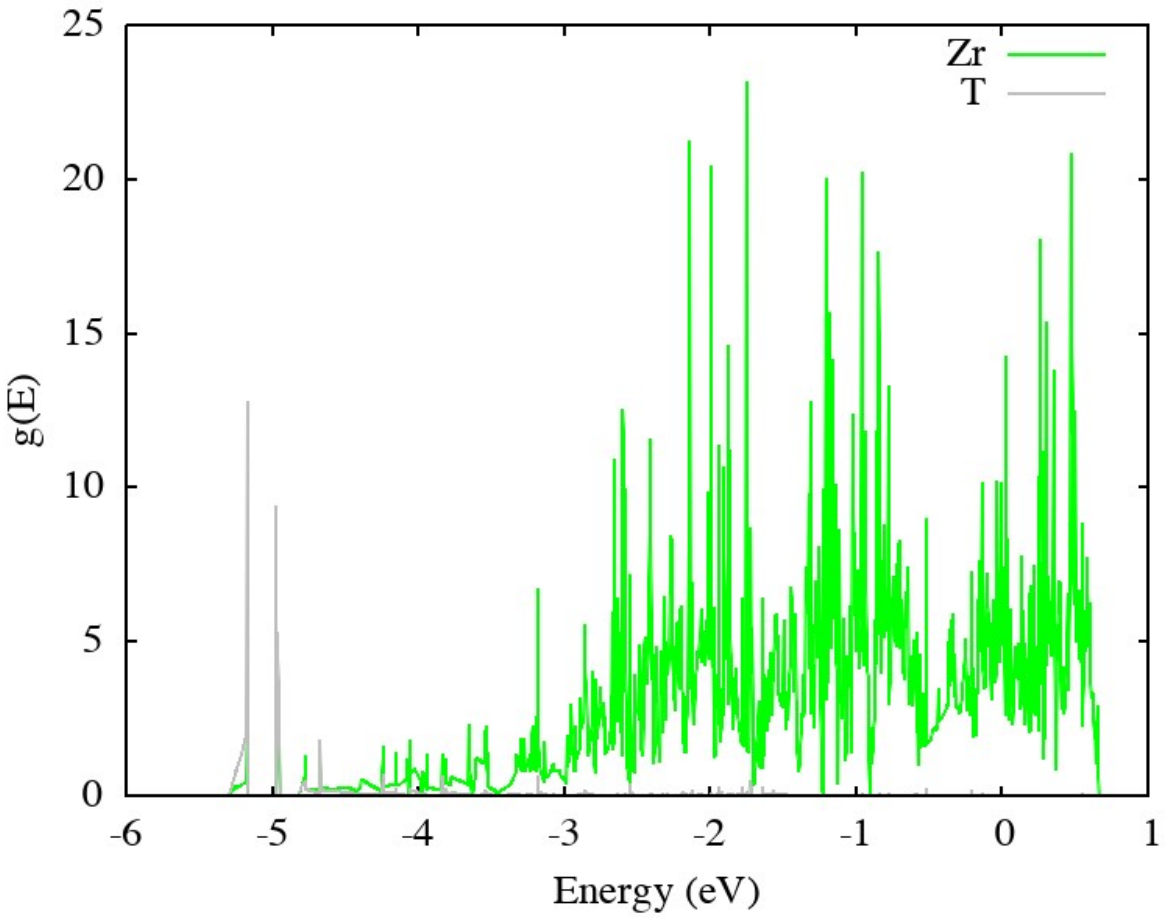

Figure S14. Projected density of states for T on an HCP site of Zr(001).

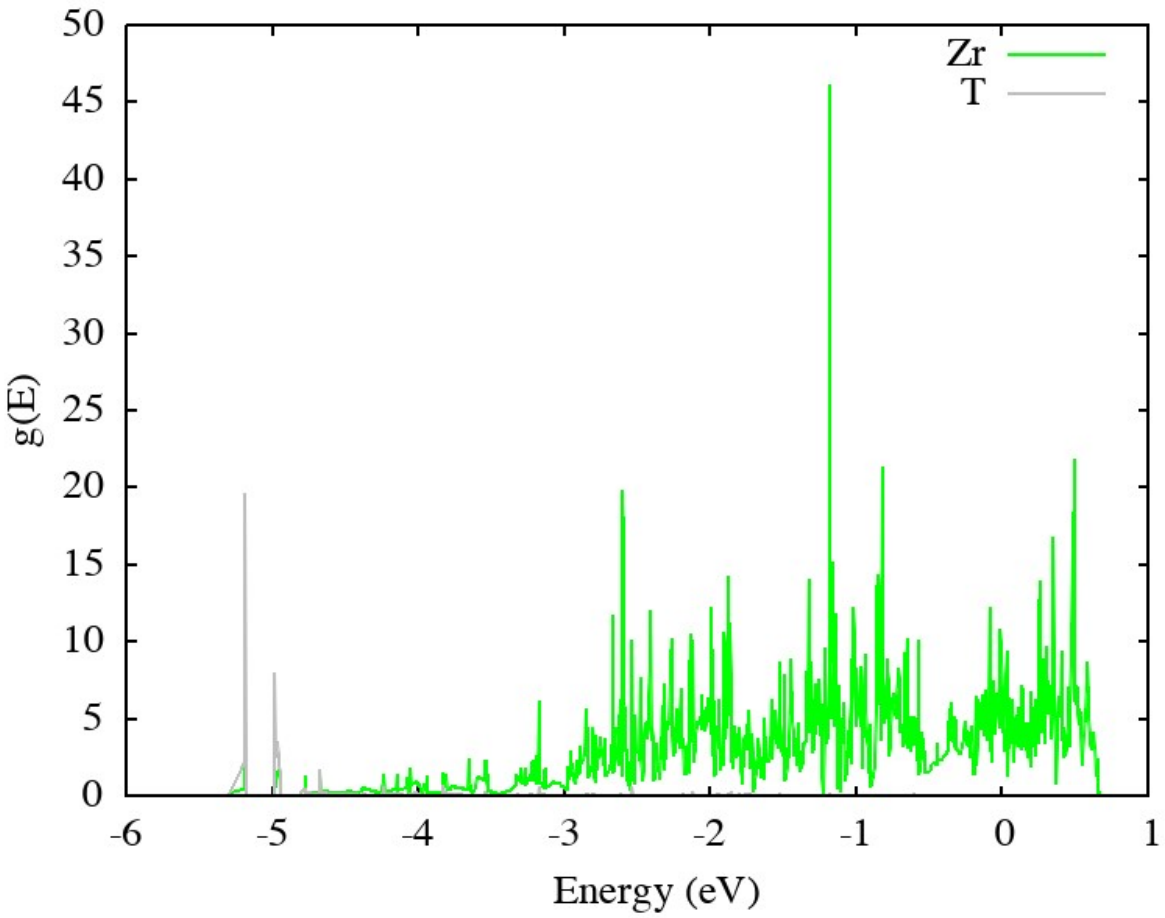

Figure S15. Projected density of states for T on a FCC site of Zr(001).

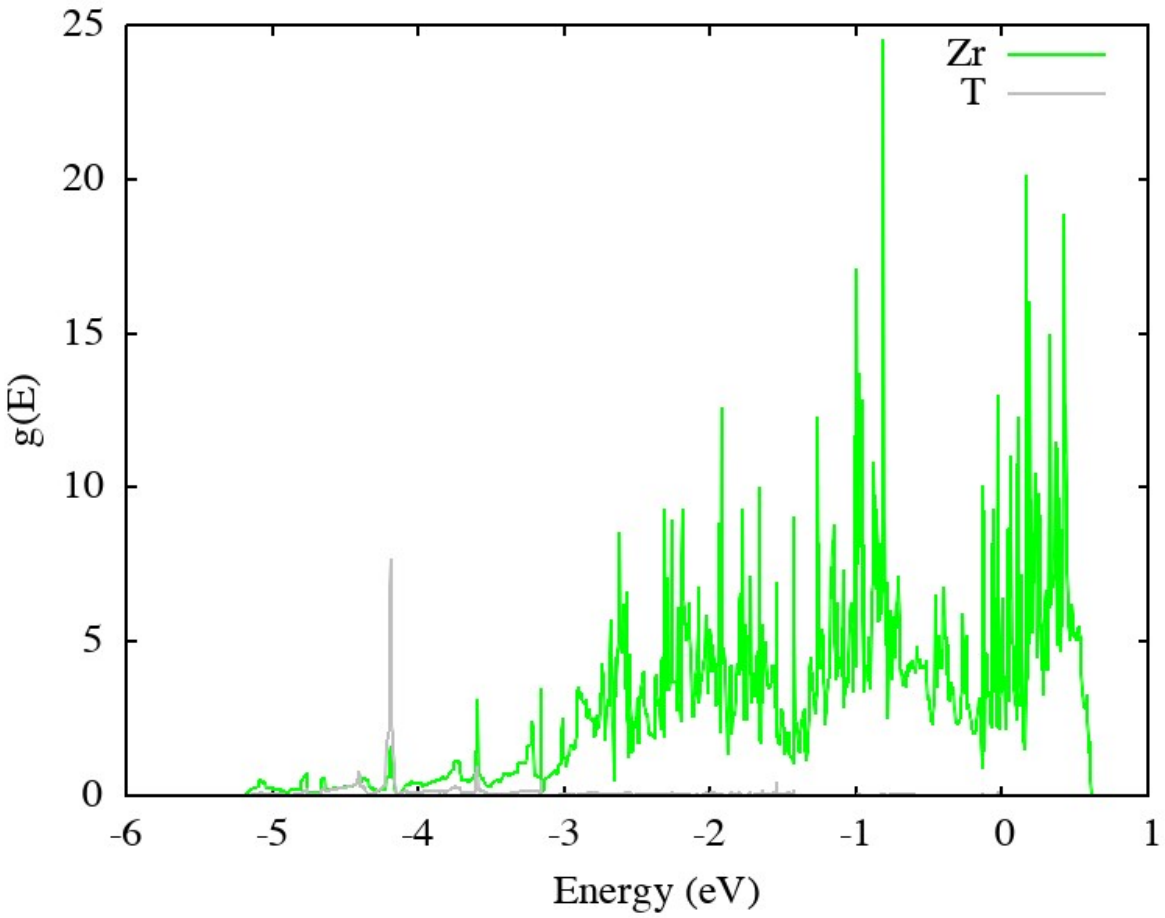

Figure S16. Projected density of states for T on an upper bridge site of Zr(100).

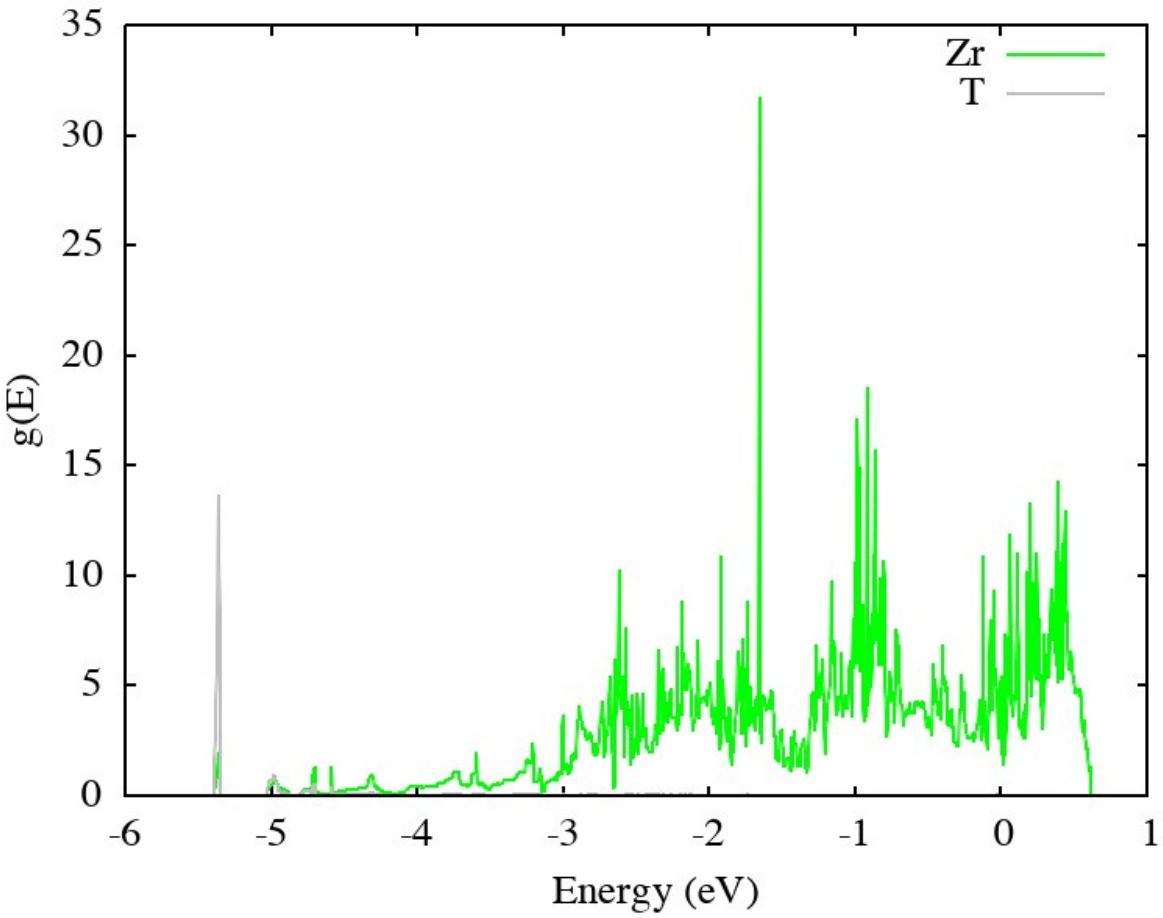

Figure S17. Projected density of states for T on a lower bridge site of Zr(100).

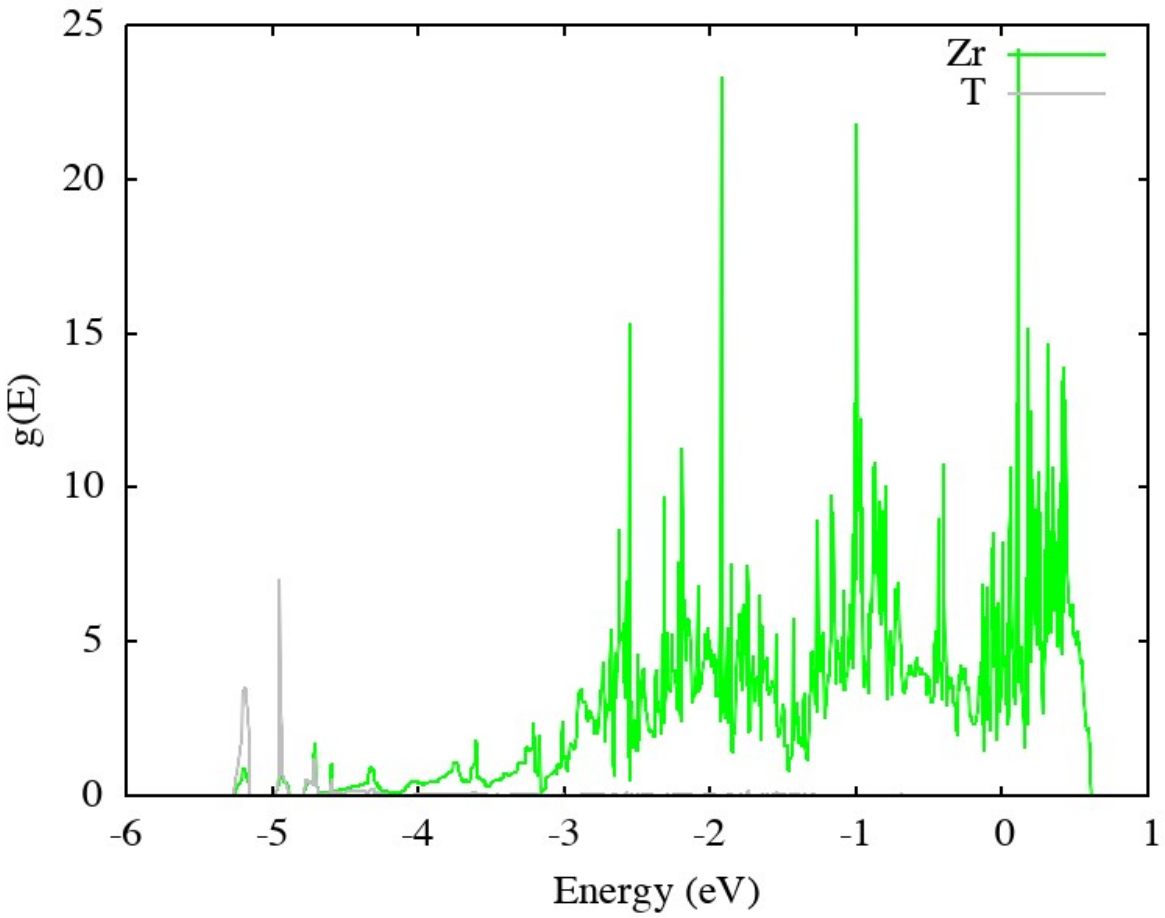

Figure S18. Projected density of states for T on a step site of Zr(100).

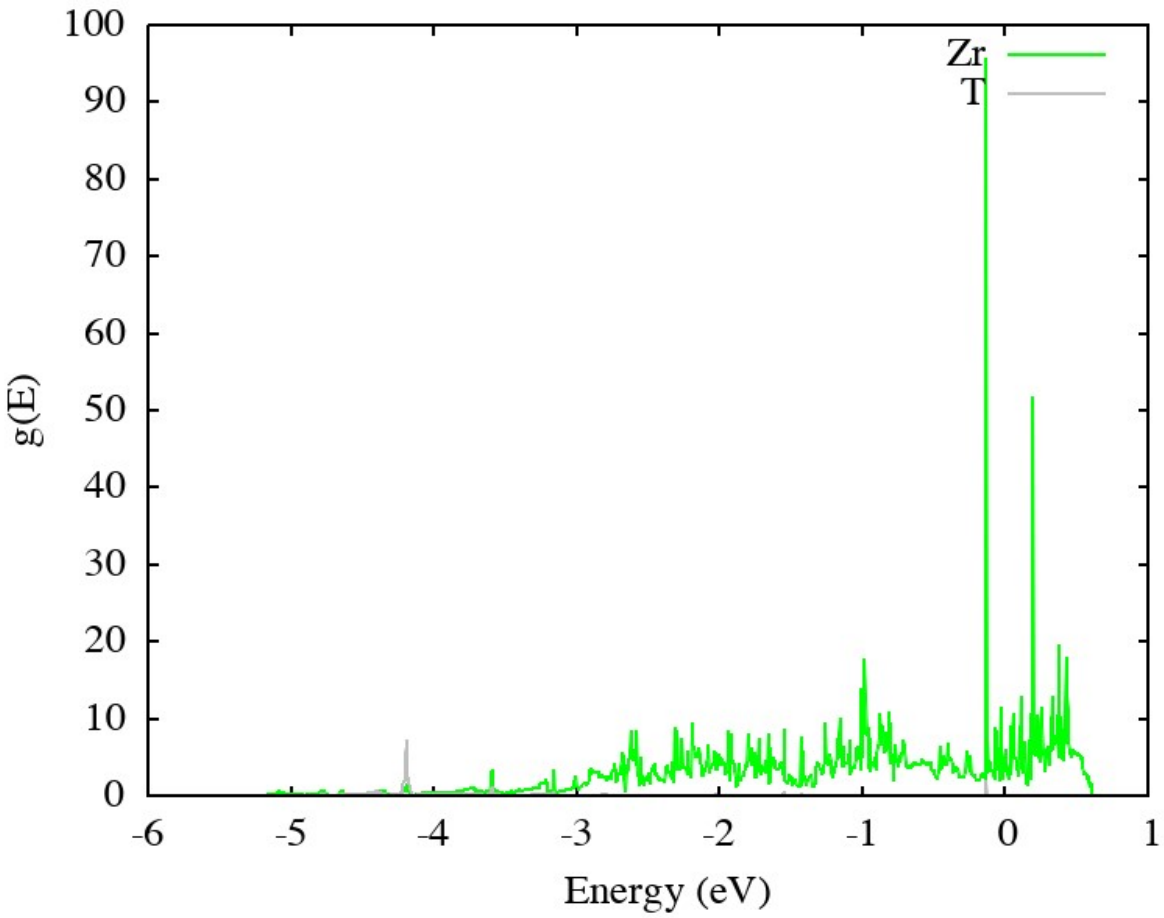

Figure S19. Projected density of states for T_2 on a top site of Zr(001).

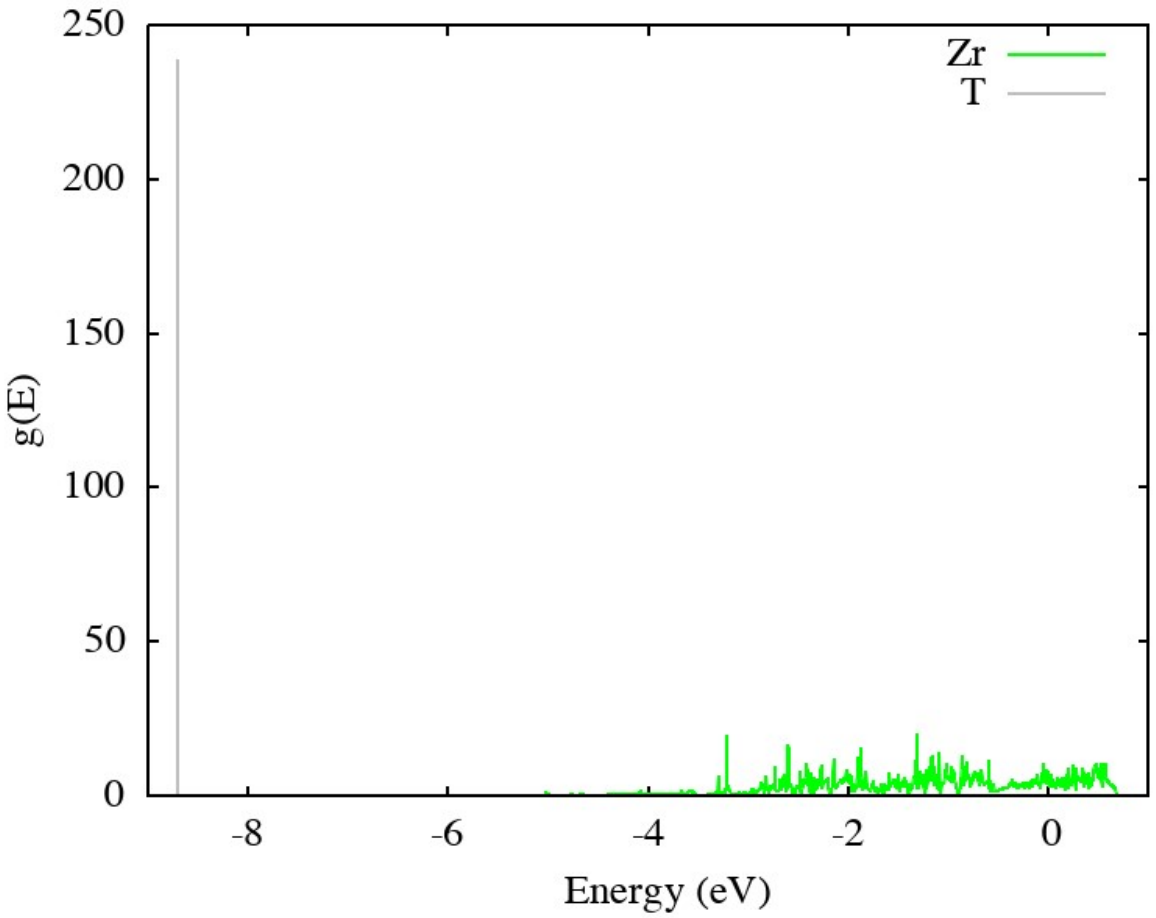

Figure S20. Projected density of states for T_2 on a FCC site of Zr(001).

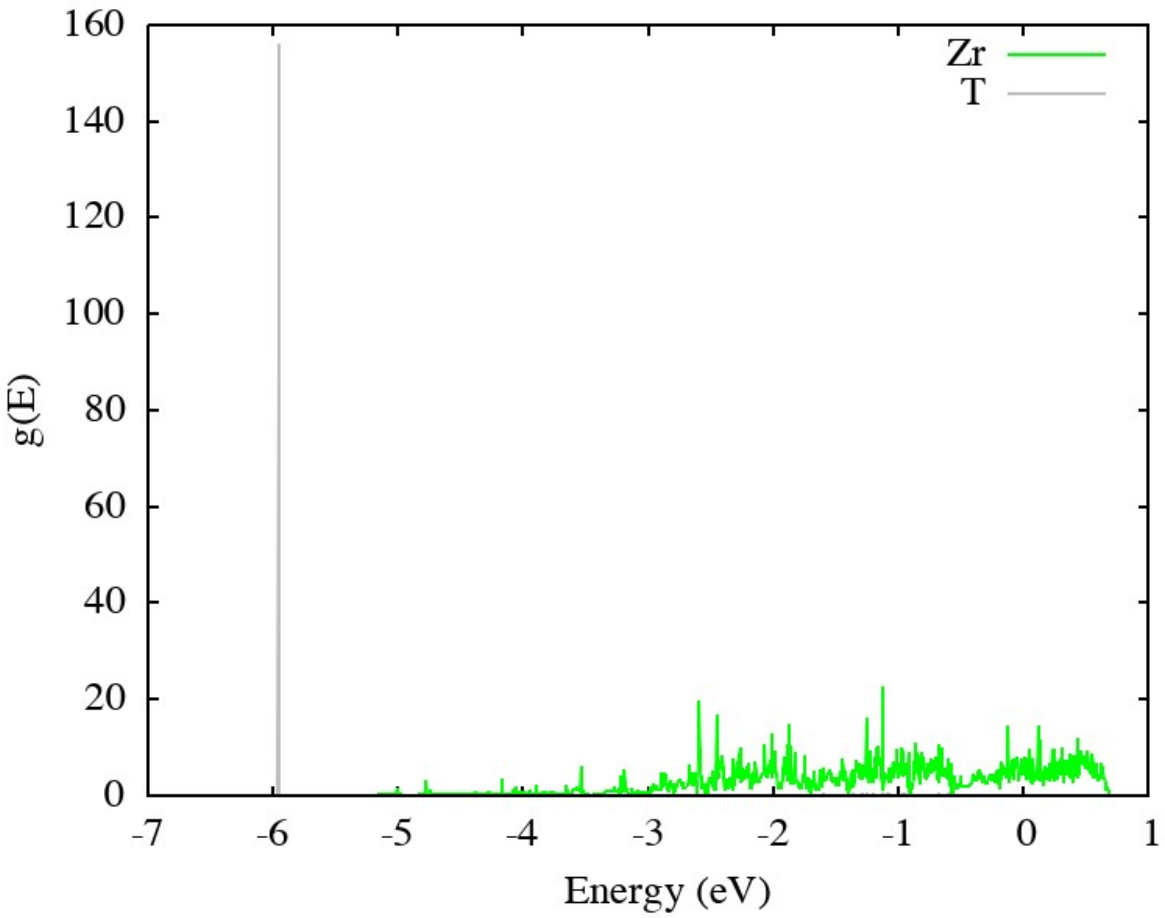

Figure S21. Projected density of states for T_2 on a top site of Zr(100).

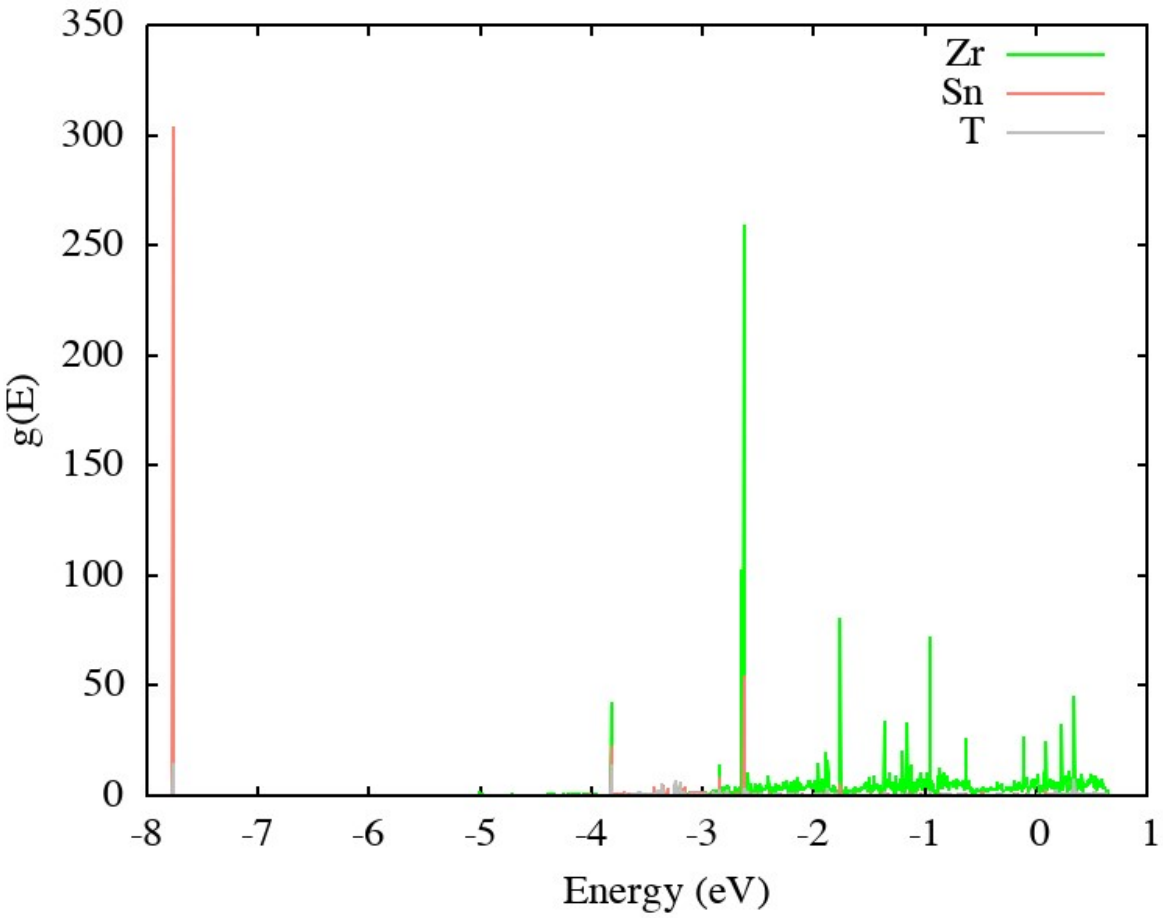

Figure S22. Projected density of states for T on a top site of Zr(001) on a surface Sn defect.

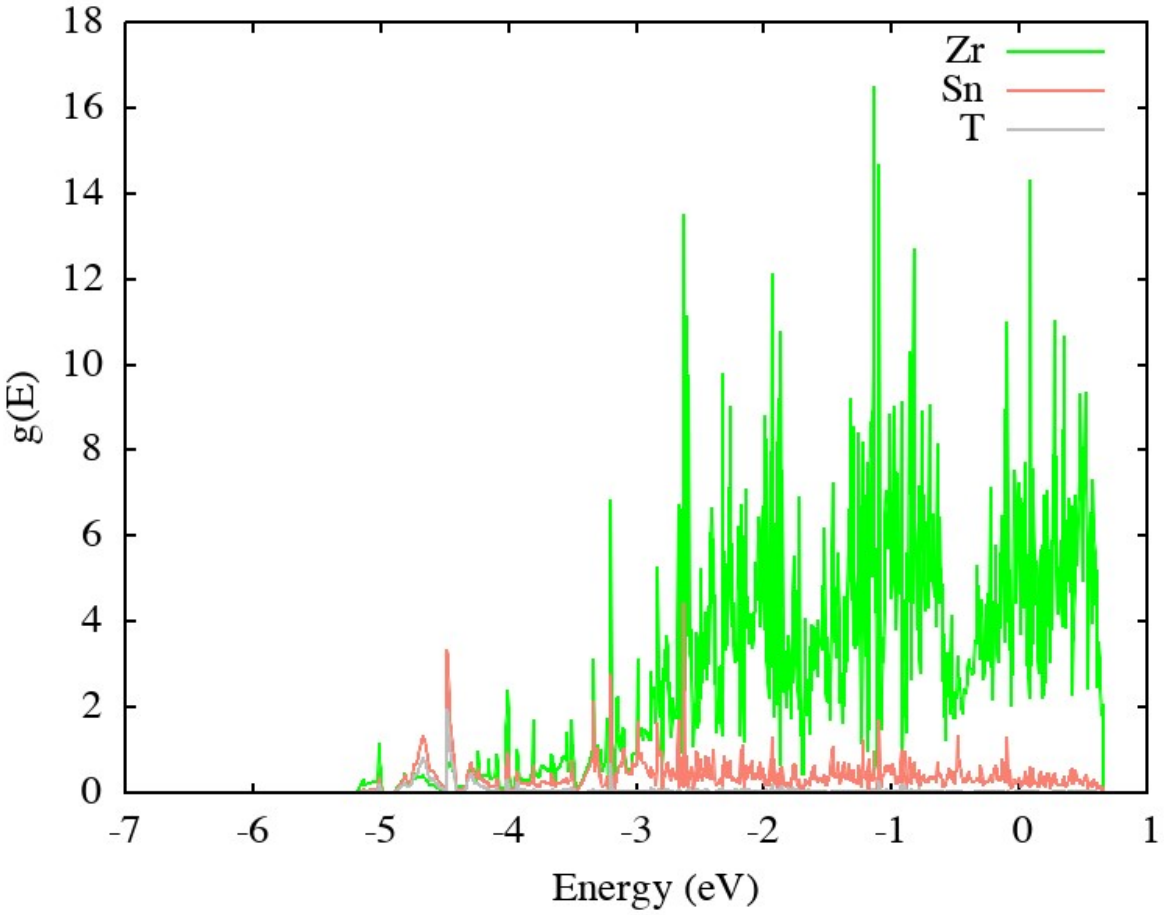

Figure S23. Projected density of states for T on a bridge site of Zr(001) on a surface Sn defect.

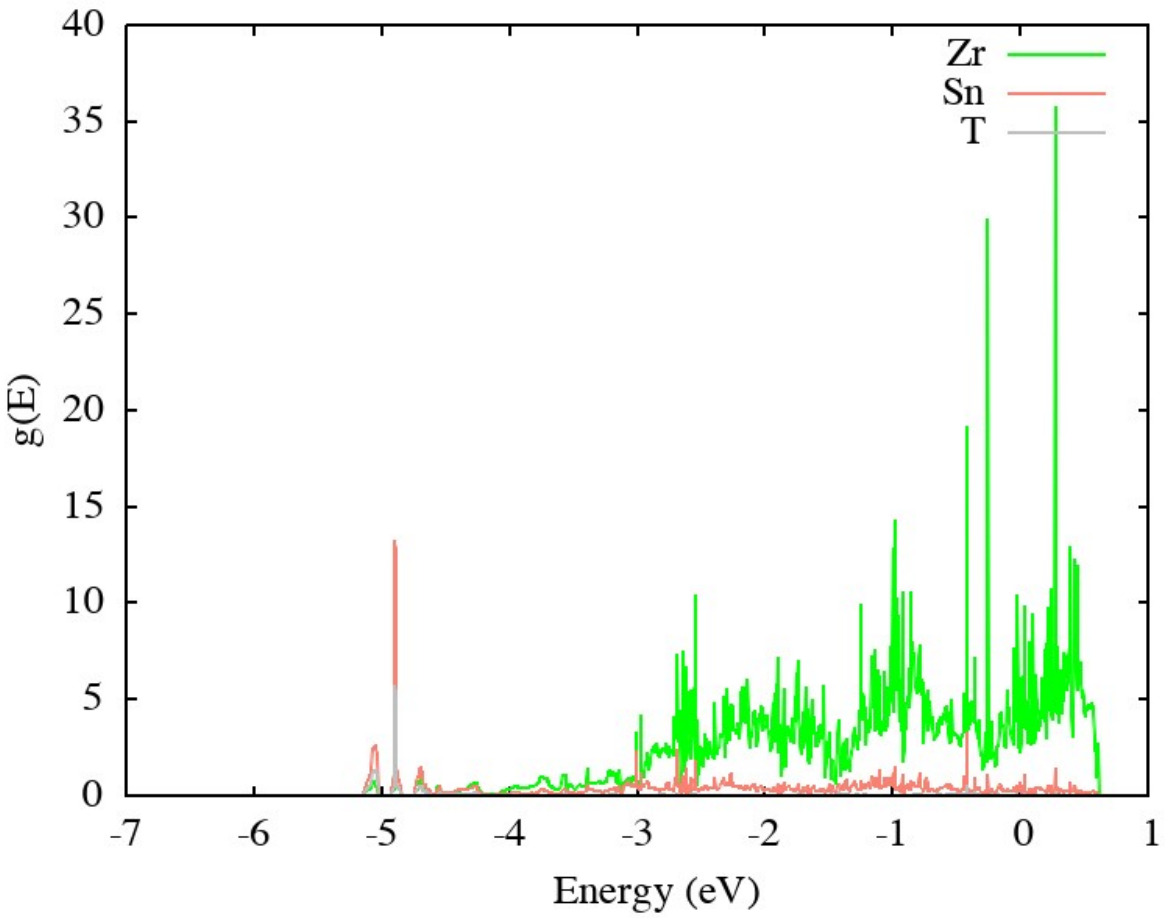

Figure S24. Projected density of states for T on an upper bridge site of Zr(100) on a surface Sn defect.

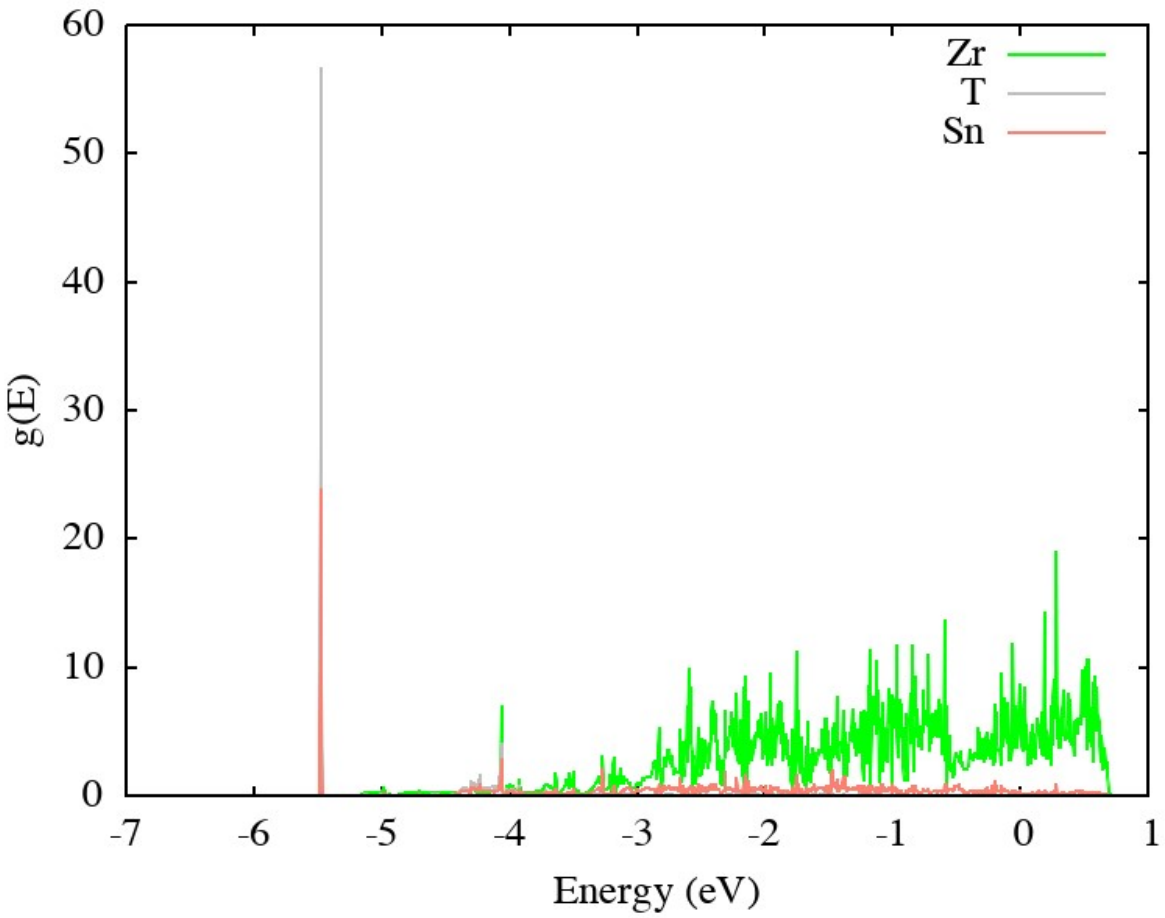

Figure S25. Projected density of states for T on a FCC site of Zr(001) on a surface Sn defect and T on a HCP site of Zr(001).

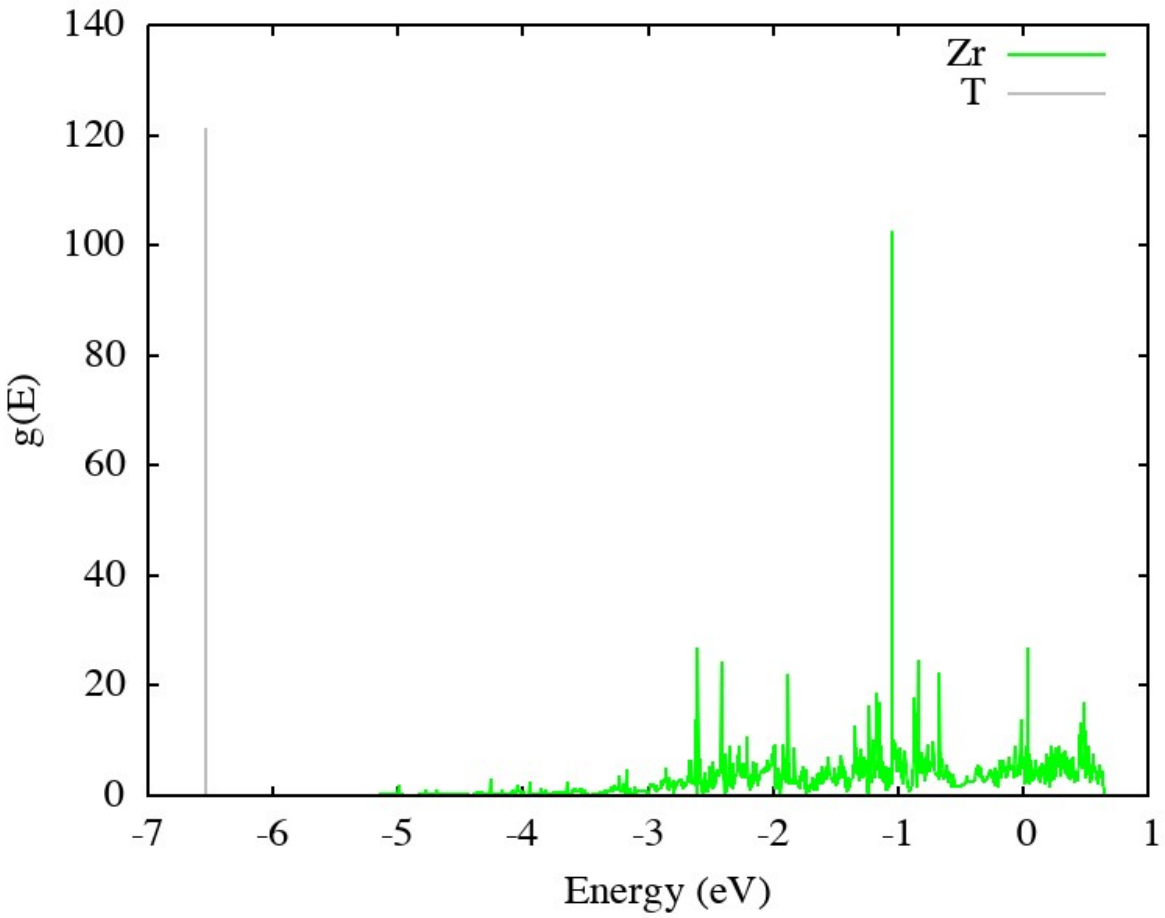

Figure S26. Projected density of states for an absorbed T in an subsurface octahedral site of Zr(001).

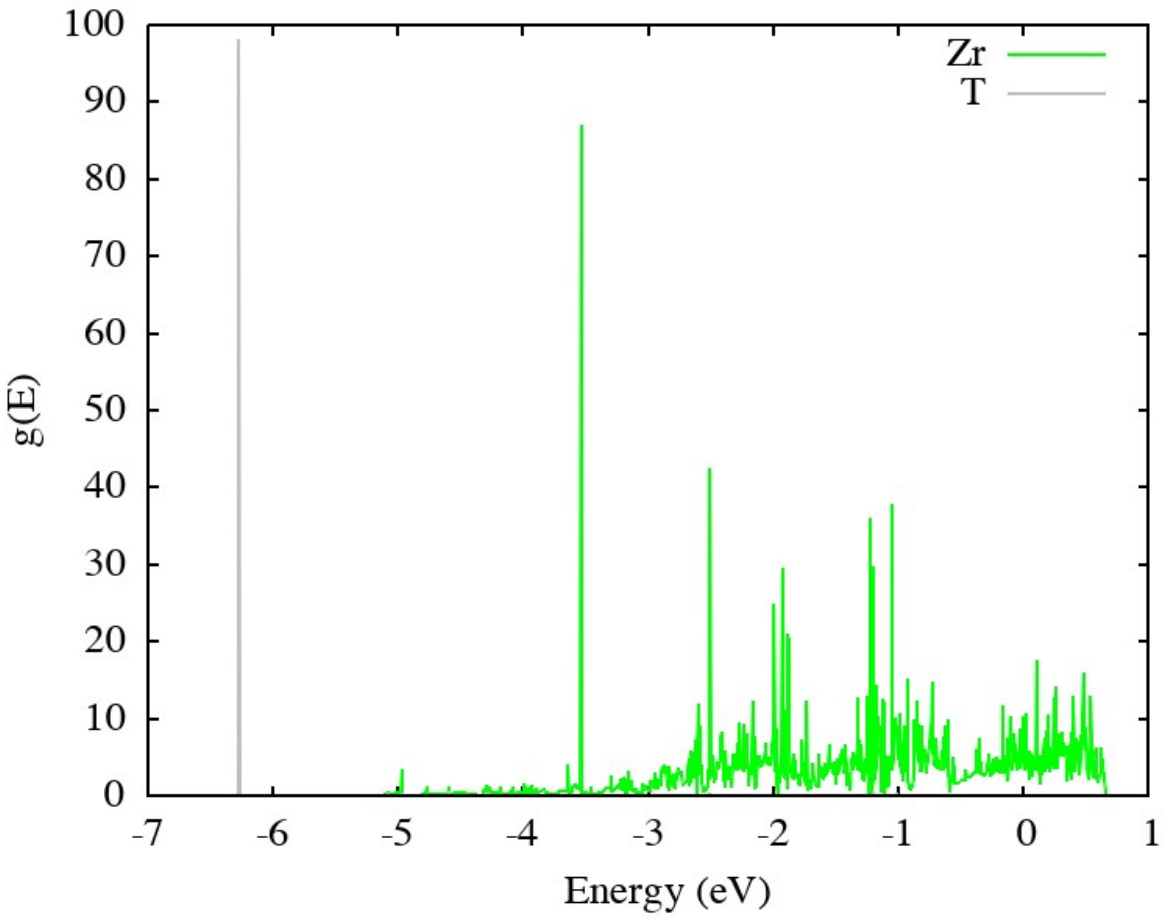

Figure S27. Projected density of states for an absorbed T in an bulk octahedral site of Zr(001).

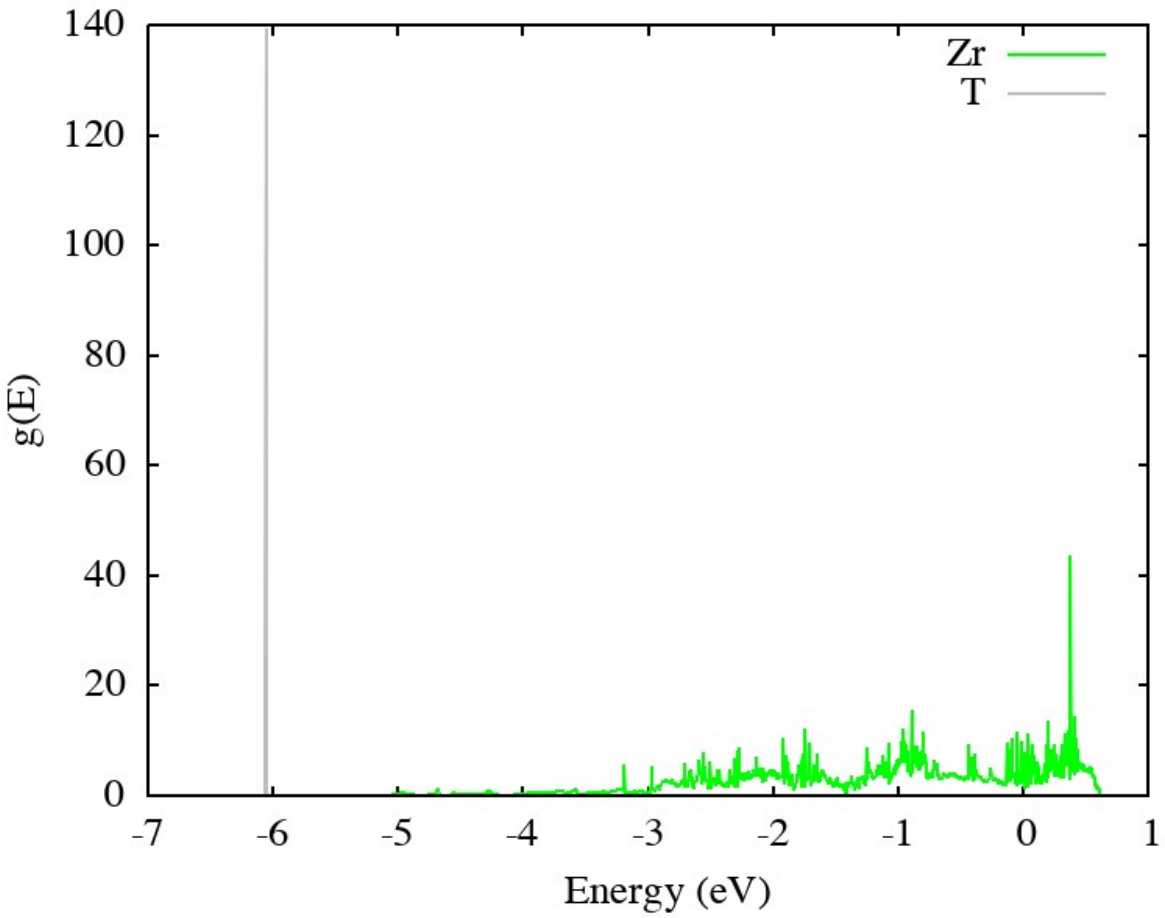

Figure S28. Projected density of states for an absorbed T in an subsurface tetrahedral site of Zr(100).

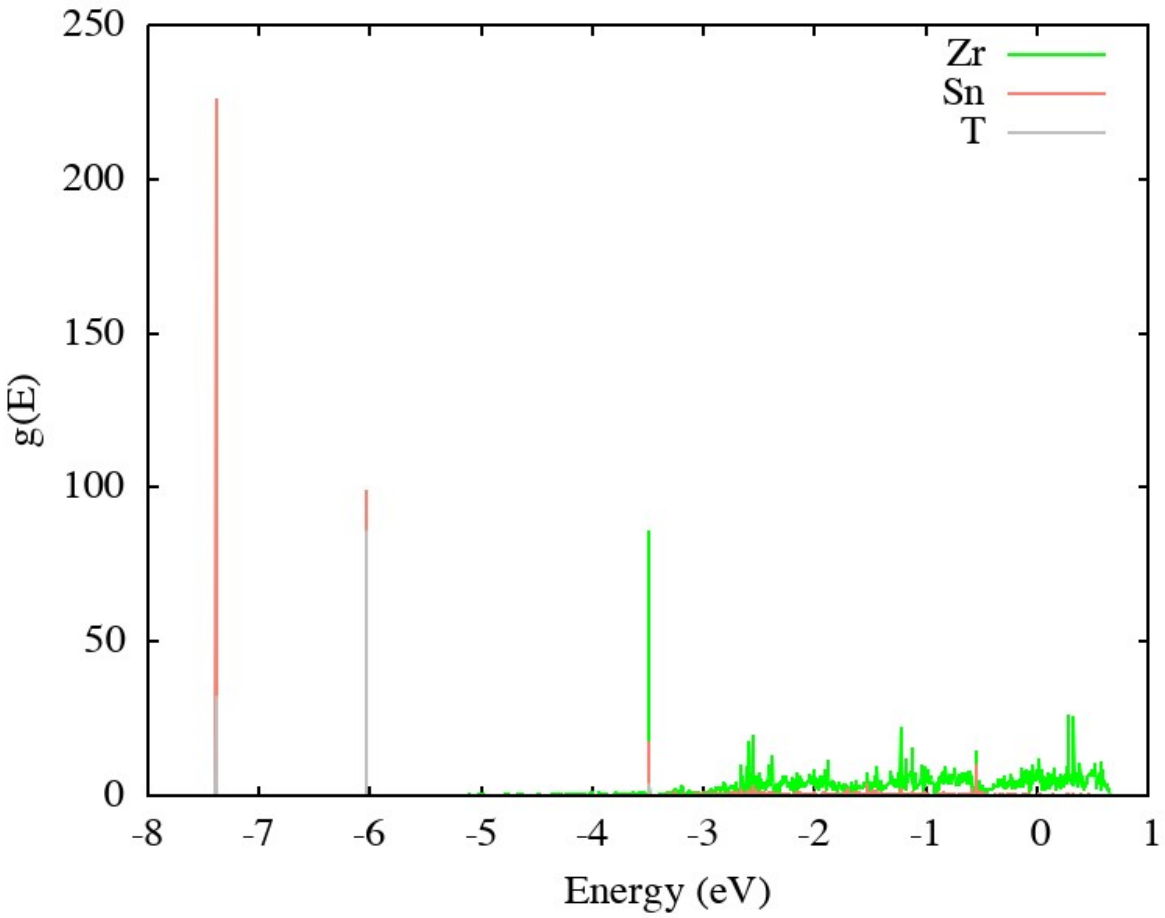

Figure S29. Projected density of states for an adsorbed T in a subsurface octahedral site on Sn of surface Sn defective Zr(001).

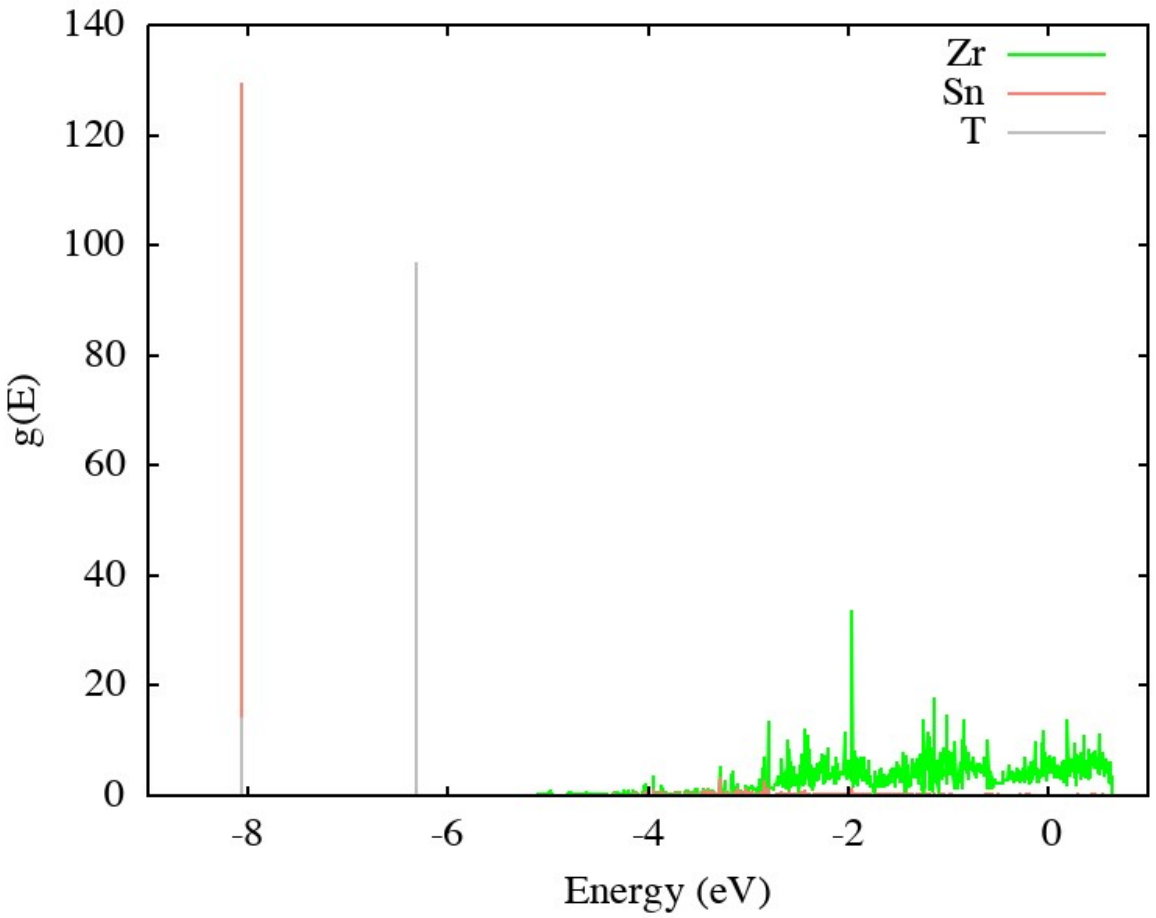

Figure S30. Projected density of states for an adsorbed T in a subsurface octahedral site on Sn of subsurface Sn defective Zr(001).

S6. Structural Coordinates

Zr(001) Bridge

```
   1.00000000000000
    16.2854995727999992    0.0000000000000000    0.0000000000000000
    -8.1427497863999996   14.1036563433000008    0.0000000000000000
     0.0000000000000000    0.0000000000000000   30.2423000335999994
   T    Zr
     1   100
Selective dynamics
Direct
  0.5340242685387580  0.5669968348405234  0.3333233898558134   T   T   T
  0.0666705933169212  0.1333294096830784  0.0442400867929322   F   F   F
  0.0666886956006394  0.1341844988575289  0.2125656176440884   T   T   T
  0.0666705933169212  0.3333294126830779  0.0442400867929322   F   F   F
  0.0670070940570611  0.3335066924456171  0.2123918636881896   T   T   T
  0.0666705933169212  0.5333294306830751  0.0442400867929322   F   F   F
  0.0666602889867818  0.5325131052967151  0.2125519756155114   T   T   T
  0.0666705933169212  0.7333294186830770  0.0442400867929322   F   F   F
  0.0656631162687660  0.7321688988916861  0.2126195606899657   T   T   T
  0.0666705933169212  0.9333294066830788  0.0442400867929322   F   F   F
  0.0657696305111131  0.9335405922202398  0.2126520416915767   T   T   T
  0.2666705813169230  0.1333294096830784  0.0442400867929322   F   F   F
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  0.2666705813169230  0.3333294126830779  0.0442400867929322   F   F   F
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  0.2666705813169230  0.5333294306830751  0.0442400867929322   F   F   F
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  0.4666705993169202  0.5333294306830751  0.0442400867929322   F   F   F
  0.4657833727872998  0.5328465580592976  0.2124412395743676   T   T   T
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0.1337309186782402	0.4663928962577839	0.2923003128537530	T	T	T
0.1333271469929400	0.6666728790070593	0.1234950372465988	F	F	F
0.1334295635262663	0.6664608026161258	0.2917202344963277	T	T	T
0.1333271469929400	0.8666728670070611	0.1234950372465988	F	F	F
0.1333406652312173	0.8666593487687844	0.2914738063364847	T	T	T
0.3333271499929396	0.0666728560070595	0.1234950372465988	F	F	F
0.3335538580763776	0.0669290746645732	0.2917281120753794	T	T	T
0.3333271499929396	0.2666728440070614	0.1234950372465988	F	F	F
0.3325865641232049	0.2650169846596503	0.2913779164015454	T	T	T
0.3333271499929396	0.4666728620070586	0.1234950372465988	F	F	F
0.3371996215408584	0.4686212836526478	0.2930037005131971	T	T	T
0.3333271499929396	0.6666728790070593	0.1234950372465988	F	F	F
0.3325134859290504	0.6674865430709482	0.2913990233336375	T	T	T
0.3333271499929396	0.8666728670070611	0.1234950372465988	F	F	F
0.3335392263838710	0.8665704504737365	0.2917202344963277	T	T	T
0.5333271679929368	0.0666728560070595	0.1234950372465988	F	F	F
0.5332839130083080	0.0666148669269434	0.2916638243958646	T	T	T
0.5333271679929368	0.2666728440070614	0.1234950372465988	F	F	F
0.5336363671603892	0.2673815334086161	0.2922958667946625	T	T	T
0.5333271679929368	0.4666728620070586	0.1234950372465988	F	F	F
0.5314117312628668	0.4685882987371282	0.2929929800331393	T	T	T
0.5333271679929368	0.6666728790070593	0.1234950372465988	F	F	F
0.5313787463473475	0.6628004074591406	0.2930037005131971	T	T	T
0.5333271679929368	0.8666728670070611	0.1234950372465988	F	F	F
0.5336071337422120	0.8662690953217622	0.2923003128537530	T	T	T
0.7333271559929386	0.0666728560070595	0.1234950372465988	F	F	F
0.7335085120870983	0.0669973224158444	0.2917925974910377	T	T	T
0.7333271559929386	0.2666728440070614	0.1234950372465988	F	F	F

0.7335324478723100 0.2664675521276944 0.2918095583220280 T T T
0.7333271559929386 0.4666728620070586 0.1234950372465988 F F F
0.7326184665913865 0.4663636628396066 0.2922958667946625 T T T
0.7333271559929386 0.6666728790070593 0.1234950372465988 F F F
0.7349830153403506 0.6674134648767944 0.2913779164015454 T T T
0.7333271559929386 0.8666728670070611 0.1234950372465988 F F F
0.7325758666913775 0.8662166949904067 0.2922870881760126 T T T
0.9333271439929405 0.0666728560070595 0.1234950372465988 F F F
0.9333256191990561 0.0666743808009450 0.2916203261046215 T T T
0.9333271439929405 0.2666728440070614 0.1234950372465988 F F F
0.9330026775841579 0.2664914879129017 0.2917925974910377 T T T
0.9333271439929405 0.4666728620070586 0.1234950372465988 F F F
0.9333851330730597 0.4667161169916875 0.2916638243958646 T T T
0.9333271439929405 0.6666728790070593 0.1234950372465988 F F F
0.9330709253354270 0.6664461709236209 0.2917281120753794 T T T
0.9333271439929405 0.8666728670070611 0.1234950372465988 F F F
0.9330006933042716 0.8665332408723727 0.2916991660181363 T T T

Zr(100) Upper Bridge

1.00000000000000
30.2854995727999992 0.0000000000000000 0.0000000000000000
-8.1427497863999996 14.1036563433000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.2423000335999994
T Zr
1 90
Selective dynamics
Direct
0.3369707845528064 0.6132235724401137 0.5833319128948322 T T T
0.0403836161104962 0.1375759132469270 0.0833333843150186 F F F
0.0403837857253251 0.1375761749917714 0.4166666478864443 F F F
0.0403837595130838 0.1375761271628164 0.7499997059658838 F F F
0.0403839047306320 0.3375760725881634 0.0833333269438725 F F F
0.0403841249569012 0.3375763038090156 0.4166666378797714 F F F
0.0403842254391478 0.3375763976028807 0.7499996387836489 F F F
0.0403837192110075 0.5375756951529098 0.0833336355039265 F F F
0.0403838829451217 0.5375759078704476 0.4166668497247272 F F F
0.0403837568668806 0.5375758539856008 0.7499999236662021 F F F
0.0403830491495825 0.7375753431503966 0.0833332937946167 F F F
0.0403831579664029 0.7375754778218777 0.4166666904606160 F F F
0.0403833047187092 0.7375756474524167 0.7499997582156439 F F F
0.0403829643395923 0.9375752265825454 0.0833334959107432 F F F
0.0403831871488904 0.9375754787448827 0.4166667221334350 F F F
0.0403831259949783 0.9375754320343788 0.7499997251739430 F F F

0.1414259212593763	0.1314848691676858	0.0833339651799321	F	F	F
0.1414268024226715	0.1314855429795259	0.4166665012805453	F	F	F
0.1414260323739569	0.1314849621537917	0.7499997154511888	F	F	F
0.1414257619797965	0.3314849728229916	0.0833342383941655	F	F	F
0.1414265444777030	0.3314859736090199	0.4166659232731007	F	F	F
0.1414257996683261	0.3314854002999468	0.7499997251055532	F	F	F
0.1414254964101573	0.5314852242310337	0.0833339579356860	F	F	F
0.1414262826673323	0.5314858984785786	0.4166659953606811	F	F	F
0.1414255198348826	0.5314849776629913	0.7499998645402428	F	F	F
0.1414254447342884	0.7314851725633673	0.0833340593776413	F	F	F
0.1414262888102229	0.7314860488381711	0.4166664065898402	F	F	F
0.1414256127011129	0.7314855528157480	0.7499996117482368	F	F	F
0.1414258462160163	0.9314850972692312	0.0833342537671911	F	F	F
0.1414266099774579	0.9314858789326834	0.4166659691123726	F	F	F
0.1414258770546937	0.9314851606315173	0.7499999667259729	F	F	F
0.2476264870270110	0.1300029192661173	0.0833333393177121	T	T	T
0.2474322696211154	0.1301375331371543	0.4163900390098390	T	T	T
0.2474315190202367	0.1301364678657349	0.7502770968537319	T	T	T
0.2474429086634451	0.3299625842874759	0.0833330174256844	T	T	T
0.2478347189104196	0.3301472408358138	0.4170703510282221	T	T	T
0.2478337992207214	0.3301460496331231	0.7495966245801297	T	T	T
0.2479602875677909	0.5304640047590797	0.0833332405639509	T	T	T
0.2467979768836663	0.5293537331089083	0.4170159905424733	T	T	T
0.2467976486585663	0.5293531744325016	0.7496501502613047	T	T	T
0.2474554377808969	0.7299830077235419	0.0833326195426078	T	T	T
0.2478316298162084	0.7304942538199755	0.4170703317469635	T	T	T
0.2478306745726277	0.7304931589127194	0.7495957609804501	T	T	T
0.2476164148107502	0.9302182365640268	0.0833332073836227	T	T	T
0.2474439560266504	0.9297419428346102	0.4163866941488605	T	T	T
0.2474438204472906	0.9297413603437336	0.7502803573884433	T	T	T
0.0752367545958847	0.0700232335656068	0.2499995996346129	F	F	F
0.0752365307345215	0.0700231091825358	0.5833341904063332	F	F	F
0.0752362489794791	0.0700229803819354	0.9166660984056705	F	F	F
0.0752365146839225	0.2700235488805234	0.2499996536057978	F	F	F
0.0752362324108873	0.2700235693189370	0.5833343393905750	F	F	F
0.0752360027057506	0.2700230919172313	0.9166658286075062	F	F	F
0.0752365237664065	0.4700239943260485	0.2499998698959160	F	F	F
0.0752362202221093	0.4700234465314281	0.5833343211008639	F	F	F
0.0752360308037581	0.4700231611422154	0.9166660379214022	F	F	F
0.0752366779530647	0.6700238190200523	0.2499996523349566	F	F	F
0.0752364422013869	0.6700239845904008	0.5833341989484992	F	F	F
0.0752362456171127	0.6700237393707056	0.9166662011996891	F	F	F
0.0752368748541201	0.8700238277755545	0.2499997053664558	F	F	F
0.0752365248966314	0.8700233739432548	0.5833342888881745	F	F	F
0.0752363583360705	0.8700230514573377	0.9166657594932914	F	F	F
0.1814910469440395	0.0685925461714811	0.2498630515561827	T	T	T

0.1814989117764649 0.0687429510110014 0.5833331531006192 T T T
0.1814897629599613 0.0685914143286889 0.9168041614249424 T T T
0.1815192896114132 0.2685904620066782 0.2502760619996306 T T T
0.1821807232448142 0.2691283447547153 0.5833330390914990 T T T
0.1815175266218320 0.2685894649614958 0.9163909839826130 T T T
0.1818936415199206 0.4691511828403380 0.2499438185649543 T T T
0.1805670042326882 0.4679028793577974 0.5833326794374231 T T T
0.1818930115371733 0.4691507961352803 0.9167231850599323 T T T
0.1815258696551250 0.6690453271865681 0.2502706015611581 T T T
0.1821795865452041 0.6696782129169796 0.5833328591893078 T T T
0.1815242878500511 0.6690433462084658 0.9163957159627469 T T T
0.1814993334614331 0.8689796046447797 0.2498671203976817 T T T
0.1815171743738364 0.8687824835151571 0.5833333764632440 T T T
0.1814983134605006 0.8689782511925307 0.9167999199455154 T T T
0.2829616340463370 0.0630467060785119 0.2501595609090673 T T T
0.2826405128590210 0.0627215299420227 0.5833339662375938 T T T
0.2829609438246165 0.0630453435843882 0.9165076687321738 T T T
0.2828955753421831 0.2630580702149480 0.2491125768705612 T T T
0.2834969555000775 0.2611926465038909 0.5833339704659253 T T T
0.2828945156673005 0.2630572738384125 0.9175542722450648 T T T
0.2827350626381251 0.4620041375653056 0.2501868601100184 T T T
0.2852800768402584 0.4694494935402326 0.5833331737553320 T T T
0.2827340402408957 0.4620037573223628 0.9164784523192352 T T T
0.2827355628820621 0.6636927160908399 0.2501980066338741 T T T
0.2852853444000413 0.6608806264926218 0.5833328905738088 T T T
0.2827345709779338 0.6636914108498976 0.9164677150077007 T T T
0.2829153573738520 0.8629508331084100 0.2491163540911952 T T T
0.2835141624988228 0.8658838628679235 0.5833334600098382 T T T
0.2829142623478934 0.8629495086900230 0.9175494990081013 T T T

Zr(100) Lower Bridge

1.00000000000000
30.2854995727999992 0.0000000000000000 0.0000000000000000
-8.1427497863999996 14.1036563433000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.2423000335999994
T Zr
1 90
Selective dynamics
Direct
0.2965573069211728 0.6755843669085588 0.4465684816233355 T T T
0.0403836161104962 0.1375759132469270 0.0833333843150186 F F F
0.0403837857253251 0.1375761749917714 0.4166666478864443 F F F
0.0403837595130838 0.1375761271628164 0.7499997059658838 F F F
0.0403839047306320 0.3375760725881634 0.0833333269438725 F F F

0.0403841249569012	0.3375763038090156	0.4166666378797714	F	F	F
0.0403842254391478	0.3375763976028807	0.7499996387836489	F	F	F
0.0403837192110075	0.5375756951529098	0.0833336355039265	F	F	F
0.0403838829451217	0.5375759078704476	0.4166668497247272	F	F	F
0.0403837568668806	0.5375758539856008	0.7499999236662021	F	F	F
0.0403830491495825	0.7375753431503966	0.0833332937946167	F	F	F
0.0403831579664029	0.7375754778218777	0.4166666904606160	F	F	F
0.0403833047187092	0.7375756474524167	0.7499997582156439	F	F	F
0.0403829643395923	0.9375752265825454	0.0833334959107432	F	F	F
0.0403831871488904	0.9375754787448827	0.4166667221334350	F	F	F
0.0403831259949783	0.9375754320343788	0.7499997251739430	F	F	F
0.1414259212593763	0.1314848691676858	0.0833339651799321	F	F	F
0.1414268024226715	0.1314855429795259	0.4166665012805453	F	F	F
0.1414260323739569	0.1314849621537917	0.7499997154511888	F	F	F
0.1414257619797965	0.3314849728229916	0.0833342383941655	F	F	F
0.1414265444777030	0.3314859736090199	0.4166659232731007	F	F	F
0.1414257996683261	0.3314854002999468	0.7499997251055532	F	F	F
0.1414254964101573	0.5314852242310337	0.0833339579356860	F	F	F
0.1414262826673323	0.5314858984785786	0.4166659953606811	F	F	F
0.1414255198348826	0.5314849776629913	0.7499998645402428	F	F	F
0.1414254447342884	0.7314851725633673	0.0833340593776413	F	F	F
0.1414262888102229	0.7314860488381711	0.4166664065898402	F	F	F
0.1414256127011129	0.7314855528157480	0.7499996117482368	F	F	F
0.1414258462160163	0.9314850972692312	0.0833342537671911	F	F	F
0.1414266099774579	0.9314858789326834	0.4166659691123726	F	F	F
0.1414258770546937	0.9314851606315173	0.7499999667259729	F	F	F
0.2475379712661100	0.1300566583813977	0.0837113804466885	T	T	T
0.2471164367936981	0.1296458438625124	0.4171893597682793	T	T	T
0.2476946931955786	0.1302000078950225	0.7499749218199897	T	T	T
0.2475860311163939	0.3296684218534830	0.0831463182386445	T	T	T
0.2479876694809139	0.3297269630779207	0.4164395360143947	T	T	T
0.2478238679792029	0.3290088934946719	0.7508529132725965	T	T	T
0.2475402192725895	0.5300176294646437	0.0820145748581599	T	T	T
0.2485265032876172	0.5315224430429757	0.4154134254704137	T	T	T
0.2466386751469268	0.5271260018649978	0.7514504751465781	T	T	T
0.2475378635323254	0.7301416343470190	0.0820200536739385	T	T	T
0.2485446543912267	0.7303589445136093	0.4154097115103877	T	T	T
0.2466270587330997	0.7313262329741348	0.7514750366507001	T	T	T
0.2476032703823139	0.9305378639039045	0.0830945699138332	T	T	T
0.2479887253111469	0.9311620502678838	0.4164216758982737	T	T	T
0.2478320443483618	0.9316562994745369	0.7508314380254294	T	T	T
0.0752367545958847	0.0700232335656068	0.2499995996346129	F	F	F
0.0752365307345215	0.0700231091825358	0.5833341904063332	F	F	F
0.0752362489794791	0.0700229803819354	0.9166660984056705	F	F	F
0.0752365146839225	0.2700235488805234	0.2499996536057978	F	F	F
0.0752362324108873	0.2700235693189370	0.5833343393905750	F	F	F

0.0752360027057506	0.2700230919172313	0.9166658286075062	F	F	F
0.0752365237664065	0.4700239943260485	0.2499998698959160	F	F	F
0.0752362202221093	0.4700234465314281	0.5833343211008639	F	F	F
0.0752360308037581	0.4700231611422154	0.9166660379214022	F	F	F
0.0752366779530647	0.6700238190200523	0.2499996523349566	F	F	F
0.0752364422013869	0.6700239845904008	0.5833341989484992	F	F	F
0.0752362456171127	0.6700237393707056	0.9166662011996891	F	F	F
0.0752368748541201	0.8700238277755545	0.2499997053664558	F	F	F
0.0752365248966314	0.8700233739432548	0.5833342888881745	F	F	F
0.0752363583360705	0.8700230514573377	0.9166657594932914	F	F	F
0.1815284207376152	0.0687997578688005	0.2502419495928176	T	T	T
0.1817733934052139	0.0690412270503128	0.5835421662503673	T	T	T
0.1812463808696102	0.0685846162135390	0.9166625629587786	T	T	T
0.1815893174585635	0.2690123632786548	0.2502338069736881	T	T	T
0.1815092704384640	0.2687374457914523	0.5833250032771947	T	T	T
0.1811634365611207	0.2683384759497892	0.9167164669386201	T	T	T
0.1813418717026478	0.4687329404419776	0.2499974473696750	T	T	T
0.1825644831748671	0.4698558803337574	0.5830469322288400	T	T	T
0.1807575695610452	0.4681103474695822	0.9169986896042269	T	T	T
0.1813567486926886	0.6684831385937454	0.2500085690813246	T	T	T
0.1825500891530623	0.6696732125275684	0.5830456161297825	T	T	T
0.1807414203593098	0.6680791652485051	0.9170123989070940	T	T	T
0.1816110395356419	0.8686960033910693	0.2501956837565681	T	T	T
0.1815427081981774	0.8688956909081770	0.5833128478476960	T	T	T
0.1811422381143620	0.8686498554183771	0.9167000549496593	T	T	T
0.2829070558883532	0.0627478864924290	0.2499339601091360	T	T	T
0.2830511091898100	0.0611997625402263	0.5835175847911451	T	T	T
0.2829737271184566	0.0638731773744250	0.9171723492957670	T	T	T
0.2829068531637797	0.2631933755544231	0.2499408855422524	T	T	T
0.2830276479674464	0.2650756550044698	0.5835726984883796	T	T	T
0.2829762521274181	0.2623106565621394	0.9171769282971467	T	T	T
0.2825759549389657	0.4631089537124536	0.2512003989526350	T	T	T
0.2825415594131852	0.4614178832800883	0.5852495629015257	T	T	T
0.2826387449818099	0.4626617858605480	0.9179796447951153	T	T	T
0.2831836605488755	0.6632375707240720	0.2406078296938133	T	T	T
0.2830498515576437	0.6631575528139636	0.5848989400376156	T	T	T
0.2830550285163481	0.6631501805749649	0.9135049353026012	T	T	T
0.2825848583199908	0.8622625808845343	0.2511810037068542	T	T	T
0.2825542287175477	0.8638530413381317	0.5852304601741521	T	T	T
0.2826477230456753	0.8628959882195516	0.9179062628694321	T	T	T

Zr(100) Step

1.00000000000000

30.2854995727999992 0.0000000000000000 0.0000000000000000

-8.1427497863999996 14.1036563433000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.2423000335999994
T Zr
1 90
Selective dynamics
Direct
0.3166355798089143 0.5943500810244280 0.5086922581486591 T T T
0.0403836161104962 0.1375759132469270 0.0833333843150186 F F F
0.0403837857253251 0.1375761749917714 0.4166666478864443 F F F
0.0403837595130838 0.1375761271628164 0.7499997059658838 F F F
0.0403839047306320 0.3375760725881634 0.0833333269438725 F F F
0.0403841249569012 0.3375763038090156 0.4166666378797714 F F F
0.0403842254391478 0.3375763976028807 0.7499996387836489 F F F
0.0403837192110075 0.5375756951529098 0.0833336355039265 F F F
0.0403838829451217 0.5375759078704476 0.4166668497247272 F F F
0.0403837568668806 0.5375758539856008 0.7499999236662021 F F F
0.0403830491495825 0.7375753431503966 0.0833332937946167 F F F
0.0403831579664029 0.7375754778218777 0.4166666904606160 F F F
0.0403833047187092 0.7375756474524167 0.7499997582156439 F F F
0.0403829643395923 0.9375752265825454 0.0833334959107432 F F F
0.0403831871488904 0.9375754787448827 0.4166667221334350 F F F
0.0403831259949783 0.9375754320343788 0.7499997251739430 F F F
0.1414259212593763 0.1314848691676858 0.0833339651799321 F F F
0.1414268024226715 0.1314855429795259 0.4166665012805453 F F F
0.1414260323739569 0.1314849621537917 0.7499997154511888 F F F
0.1414257619797965 0.3314849728229916 0.0833342383941655 F F F
0.1414265444777030 0.3314859736090199 0.4166659232731007 F F F
0.1414257996683261 0.3314854002999468 0.7499997251055532 F F F
0.1414254964101573 0.5314852242310337 0.0833339579356860 F F F
0.1414262826673323 0.5314858984785786 0.4166659953606811 F F F
0.1414255198348826 0.5314849776629913 0.7499998645402428 F F F
0.1414254447342884 0.7314851725633673 0.0833340593776413 F F F
0.1414262888102229 0.7314860488381711 0.4166664065898402 F F F
0.1414256127011129 0.7314855528157480 0.7499996117482368 F F F
0.1414258462160163 0.9314850972692312 0.0833342537671911 F F F
0.1414266099774579 0.9314858789326834 0.4166659691123726 F F F
0.1414258770546937 0.9314851606315173 0.7499999667259729 F F F
0.2476694797716457 0.1300013925950592 0.0841021802626461 T T T
0.2473455226724244 0.1300577389230715 0.4173318909304151 T T T
0.2472842901102693 0.1298210648853601 0.7507371517089116 T T T
0.2472349927236282 0.3297702353595663 0.0836681479101872 T T T
0.2469196144589795 0.3295136834246745 0.4170188172790525 T T T
0.2474135763508709 0.3293731150764054 0.7511129684991473 T T T
0.2475015255975057 0.5300086026575886 0.0829244669751032 T T T
0.2536696968018023 0.5357135134462293 0.4168954593597274 T T T
0.2472604874799839 0.5297970957577114 0.7484255425037157 T T T

0.2472510401199553	0.7297489605732675	0.0836632458517740	T	T	T
0.2469234272029003	0.7294071935824977	0.4169957159209924	T	T	T
0.2474344430459401	0.7305096933941838	0.7510803506548508	T	T	T
0.2476794036872083	0.9302708430169125	0.0841037592800830	T	T	T
0.2473648259545298	0.9296313139220106	0.4173336169415722	T	T	T
0.2473147028934486	0.9297698676375964	0.7507342390414538	T	T	T
0.0752367545958847	0.0700232335656068	0.2499995996346129	F	F	F
0.0752365307345215	0.0700231091825358	0.5833341904063332	F	F	F
0.0752362489794791	0.0700229803819354	0.9166660984056705	F	F	F
0.0752365146839225	0.2700235488805234	0.2499996536057978	F	F	F
0.0752362324108873	0.2700235693189370	0.5833343393905750	F	F	F
0.0752360027057506	0.2700230919172313	0.9166658286075062	F	F	F
0.0752365237664065	0.4700239943260485	0.2499998698959160	F	F	F
0.0752362202221093	0.4700234465314281	0.5833343211008639	F	F	F
0.0752360308037581	0.4700231611422154	0.9166660379214022	F	F	F
0.0752366779530647	0.6700238190200523	0.2499996523349566	F	F	F
0.0752364422013869	0.6700239845904008	0.5833341989484992	F	F	F
0.0752362456171127	0.6700237393707056	0.9166662011996891	F	F	F
0.0752368748541201	0.8700238277755545	0.2499997053664558	F	F	F
0.0752365248966314	0.8700233739432548	0.5833342888881745	F	F	F
0.0752363583360705	0.8700230514573377	0.9166657594932914	F	F	F
0.1812239589274163	0.0684766343169415	0.2502213563152456	T	T	T
0.1812646488093306	0.0684263135093747	0.5836056420949939	T	T	T
0.1815576323852597	0.0685961162066956	0.9170327210805013	T	T	T
0.1812065201730192	0.2685282550111299	0.2500255321741598	T	T	T
0.1817359164142707	0.2685135743440622	0.5843087324833802	T	T	T
0.1816375441734267	0.2687009734574554	0.9168814012789811	T	T	T
0.1813380524910857	0.4686217834500423	0.2509075040346468	T	T	T
0.1815974517568200	0.4688877258146314	0.5811659332384103	T	T	T
0.1811968303938135	0.4685228584491832	0.9160493730367505	T	T	T
0.1811961379584794	0.6684476238031111	0.2500209116702466	T	T	T
0.1817458805811939	0.6695418318192896	0.5843045631640033	T	T	T
0.1816445604571231	0.6691522414739406	0.9168694502318158	T	T	T
0.1812244848417299	0.8685718447985175	0.2502256638175237	T	T	T
0.1812735201982678	0.8687430564779403	0.5836121597632866	T	T	T
0.1815682259301067	0.8690836975397142	0.9170260784536090	T	T	T
0.2827527847917809	0.0628205115163895	0.2510177610957760	T	T	T
0.2824706861977322	0.0625845820357814	0.5846584454196788	T	T	T
0.2829594516916318	0.0630243902055268	0.9182909225708549	T	T	T
0.2825700585001395	0.2620259256459593	0.2512884640334944	T	T	T
0.2832326472096406	0.2627144725674247	0.5854575470809531	T	T	T
0.2829563329702625	0.2619288996442750	0.9187111424922512	T	T	T
0.2826641066869363	0.4642617321639055	0.2491307968548767	T	T	T
0.2830406749710940	0.4629555260358764	0.5795933107985057	T	T	T
0.2825552743381458	0.4636659033541889	0.9158037925345676	T	T	T
0.2826579080366246	0.6612389577273581	0.2491423807665017	T	T	T

0.2830404074500430 0.6633024555239648 0.5795575772417764 T T T
0.2825603099820376 0.6616840697278319 0.9157858165146670 T T T
0.2825876045093491 0.8633402843786596 0.2512867179075853 T T T
0.2832551733377129 0.8639130652903307 0.5854209950403737 T T T
0.2829768149001680 0.8641556004645580 0.9186873066761354 T T T

Zr(001) Subsurface Octahedral

T Zr
1.00000000000000
16.2854995727999992 0.0000000000000000 0.0000000000000000
-8.1427497863999996 14.1036563433000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.2423000335999994
T Zr
1 100
Selective dynamics
Direct
0.3999920146652107 0.5999922792254054 0.2524567023778374 T T T
0.0666705933169212 0.1333294096830784 0.0442400867929322 F F F
0.0642791105499155 0.1334460066803885 0.2125674230116481 T T T
0.0666705933169212 0.3333294126830779 0.0442400867929322 F F F
0.0683419881170311 0.3344262874429307 0.2123774477142169 T T T
0.0666705933169212 0.5333294306830751 0.0442400867929322 F F F
0.0683566857905751 0.5339392015349905 0.2123569484679502 T T T
0.0666705933169212 0.7333294186830770 0.0442400867929322 F F F
0.0644130589270442 0.7309749594500938 0.2125687806752060 T T T
0.0666705933169212 0.9333294066830788 0.0442400867929322 F F F
0.0666866658950450 0.9332982780696258 0.2125927056777017 T T T
0.2666705813169230 0.1333294096830784 0.0442400867929322 F F F
0.2690387367497295 0.1334696895656312 0.2125552447966148 T T T
0.2666705813169230 0.3333294126830779 0.0442400867929322 F F F
0.2636783531239498 0.3274376110656124 0.2119759021378469 T T T
0.2666705813169230 0.5333294306830751 0.0442400867929322 F F F
0.2619847369940528 0.5309858898691213 0.2131519304947079 T T T
0.2666705813169230 0.7333294186830770 0.0442400867929322 F F F
0.2637399152455316 0.7362522302946908 0.2119367397475278 T T T
0.2666705813169230 0.9333294066830788 0.0442400867929322 F F F
0.2690146445330941 0.9355802090685850 0.2125693752230599 T T T
0.4666705993169202 0.1333294096830784 0.0442400867929322 F F F
0.4676422331522145 0.1338249317504310 0.2126803725614123 T T T
0.4666705993169202 0.3333294126830779 0.0442400867929322 F F F
0.4660451423090750 0.3344045641015807 0.2123698140025155 T T T
0.4666705993169202 0.5333294306830751 0.0442400867929322 F F F
0.4689742958820945 0.5310027552740852 0.2131299603867790 T T T
0.4666705993169202 0.7333294186830770 0.0442400867929322 F F F

0.4689988814311641	0.7379943696654243	0.2131496115430798	T	T	T
0.4666705993169202	0.9333294066830788	0.0442400867929322	F	F	F
0.4660463716673718	0.9316290739084138	0.2123574266490686	T	T	T
0.6666706163169209	0.1333294096830784	0.0442400867929322	F	F	F
0.6657527305165638	0.1315595353531377	0.2124112795092797	T	T	T
0.6666706163169209	0.3333294126830779	0.0442400867929322	F	F	F
0.6657481675439655	0.3342327051254427	0.2124296959730370	T	T	T
0.6666706163169209	0.5333294306830751	0.0442400867929322	F	F	F
0.6655773137572339	0.5339430872129423	0.2123693488658809	T	T	T
0.6666706163169209	0.7333294186830770	0.0442400867929322	F	F	F
0.6725517817033358	0.7363081030435230	0.2119773709595832	T	T	T
0.6666706163169209	0.9333294066830788	0.0442400867929322	F	F	F
0.6655618895844649	0.9316433849918625	0.2123773905655133	T	T	T
0.8666706043169228	0.1333294096830784	0.0442400867929322	F	F	F
0.8661138695737970	0.1338671711618499	0.2126740684916235	T	T	T
0.8666706043169228	0.3333294126830779	0.0442400867929322	F	F	F
0.8684258398524927	0.3342353236416400	0.2124125944927535	T	T	T
0.8666706043169228	0.5333294306830751	0.0442400867929322	F	F	F
0.8661607608511230	0.5323449834752623	0.2126798129013787	T	T	T
0.8666706043169228	0.7333294186830770	0.0442400867929322	F	F	F
0.8665198963393044	0.7309507598181846	0.2125542022487479	T	T	T
0.8666706043169228	0.9333294066830788	0.0442400867929322	F	F	F
0.8665435157482189	0.9357052840358460	0.2125694877791637	T	T	T
0.1333271469929400	0.0666728560070595	0.1234950372465988	F	F	F
0.1340598451353719	0.0682332952356350	0.2908169103574976	T	T	T
0.1333271469929400	0.2666728440070614	0.1234950372465988	F	F	F
0.1328700802934613	0.2664313455291513	0.2925111927866865	T	T	T
0.1333271469929400	0.4666728620070586	0.1234950372465988	F	F	F
0.1300352540429558	0.4650400081909146	0.2931970881259072	T	T	T
0.1333271469929400	0.6666728790070593	0.1234950372465988	F	F	F
0.1329272504207962	0.6664448579993852	0.2924765233092247	T	T	T
0.1333271469929400	0.8666728670070611	0.1234950372465988	F	F	F
0.1340996720011455	0.8658957211930883	0.2908647289592880	T	T	T
0.3333271499929396	0.0666728560070595	0.1234950372465988	F	F	F
0.3341233788984262	0.0670877816702966	0.2925014968415098	T	T	T
0.3333271499929396	0.2666728440070614	0.1234950372465988	F	F	F
0.3335419657589402	0.2664422581876753	0.2925014592124082	T	T	T
0.3333271499929396	0.4666728620070586	0.1234950372465988	F	F	F
0.3305169864884137	0.4610567717464699	0.2906407499856619	T	T	T
0.3333271499929396	0.6666728790070593	0.1234950372465988	F	F	F
0.3305102020290029	0.6694803848200672	0.2906364358086076	T	T	T
0.3333271499929396	0.8666728670070611	0.1234950372465988	F	F	F
0.3335452201755207	0.8670669469846450	0.2924776091915398	T	T	T
0.5333271679929368	0.0666728560070595	0.1234950372465988	F	F	F
0.5327207725498465	0.0655558224769278	0.2918020646217337	T	T	T
0.5333271679929368	0.2666728440070614	0.1234950372465988	F	F	F

0.5327162641273276 0.2671579645650611 0.2918254746291896 T T T
0.5333271679929368 0.4666728620070586 0.1234950372465988 F F F
0.5349410135053879 0.4650447559372337 0.2931775650298766 T T T
0.5333271679929368 0.6666728790070593 0.1234950372465988 F F F
0.5389263515831109 0.6694636671212941 0.2906390278338574 T T T
0.5333271679929368 0.8666728670070611 0.1234950372465988 F F F
0.5349450192839524 0.8699475452394215 0.2931949251822017 T T T
0.7333271559929386 0.0666728560070595 0.1234950372465988 F F F
0.7327865747131311 0.0655959667093515 0.2918187589147630 T T T
0.7333271559929386 0.2666728440070614 0.1234950372465988 F F F
0.7333171810135104 0.2666683677722643 0.2903950101140051 T T T
0.7333271559929386 0.4666728620070586 0.1234950372465988 F F F
0.7328278772660491 0.4672718528170259 0.2918220355801458 T T T
0.7333271559929386 0.6666728790070593 0.1234950372465988 F F F
0.7335508038435409 0.6664476372662049 0.2925007714309012 T T T
0.7333271559929386 0.8666728670070611 0.1234950372465988 F F F
0.7335542525153791 0.8671146018604229 0.2925111339812042 T T T
0.9333271439929405 0.0666728560070595 0.1234950372465988 F F F
0.9328582206774703 0.0671285423722788 0.2925382221344677 T T T
0.9333271439929405 0.2666728440070614 0.1234950372465988 F F F
0.9343913800894746 0.2671978223022488 0.2918182732750565 T T T
0.9333271439929405 0.4666728620070586 0.1234950372465988 F F F
0.9344325093652784 0.4672710363437481 0.2918014168792728 T T T
0.9333271439929405 0.6666728790070593 0.1234950372465988 F F F
0.9329044213151385 0.6658705312158467 0.2924987113220415 T T T
0.9333271439929405 0.8666728670070611 0.1234950372465988 F F F
0.9317550023212076 0.8659261725531526 0.2908192570469738 T T T

Zr(001)Bulk Octahedral

0001_4_layer
1.00000000000000
16.2854995727999992 0.0000000000000000 0.0000000000000000
-8.1427497863999996 14.1036563433000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.2423000335999994
T Zr
1 100
Selective dynamics
Direct
0.3999606007914167 0.5999825760744761 0.1679155619067597 T T T
0.0666705933169212 0.1333294096830784 0.0442400867929322 F F F
0.0655033629332022 0.1333084662987424 0.2126042963168437 T T T
0.0666705933169212 0.3333294126830779 0.0442400867929322 F F F
0.0674881792508980 0.3352802959654917 0.2130257396659694 T T T
0.0666705933169212 0.5333294306830751 0.0442400867929322 F F F

0.0674475465669257	0.5322340791836979	0.2130302733828418	T	T	T
0.0666705933169212	0.7333294186830770	0.0442400867929322	F	F	F
0.0655298440741376	0.7322279192937424	0.2125808678393795	T	T	T
0.0666705933169212	0.9333294066830788	0.0442400867929322	F	F	F
0.0666562096495855	0.9332690648170066	0.2123947044205047	T	T	T
0.2666705813169230	0.1333294096830784	0.0442400867929322	F	F	F
0.2676994176405605	0.1333414081762592	0.2125678817222302	T	T	T
0.2666705813169230	0.3333294126830779	0.0442400867929322	F	F	F
0.2656203105180498	0.3312517631017112	0.2119473249887601	T	T	T
0.2666705813169230	0.5333294306830751	0.0442400867929322	F	F	F
0.2632444435703791	0.5316656572300207	0.2127084973659472	T	T	T
0.2666705813169230	0.7333294186830770	0.0442400867929322	F	F	F
0.2655967375154578	0.7343577852042625	0.2119481868102043	T	T	T
0.2666705813169230	0.9333294066830788	0.0442400867929322	F	F	F
0.2677019074777428	0.9344022579251847	0.2125837702287961	T	T	T
0.4666705993169202	0.1333294096830784	0.0442400867929322	F	F	F
0.4661885271386725	0.1331083435888573	0.2128078459024643	T	T	T
0.4666705993169202	0.3333294126830779	0.0442400867929322	F	F	F
0.4677035122415993	0.3351864867381095	0.2130055214122006	T	T	T
0.4666705993169202	0.5333294306830751	0.0442400867929322	F	F	F
0.4683025234007634	0.5316468633006127	0.2127162743408704	T	T	T
0.4666705993169202	0.7333294186830770	0.0442400867929322	F	F	F
0.4682741192493359	0.7366790703621617	0.2127058026453890	T	T	T
0.4666705993169202	0.9333294066830788	0.0442400867929322	F	F	F
0.4677092709286758	0.9324935053575713	0.2130310627778684	T	T	T
0.6666706163169209	0.1333294096830784	0.0442400867929322	F	F	F
0.6671599475531179	0.1343568053699210	0.2124368518735401	T	T	T
0.6666706163169209	0.3333294126830779	0.0442400867929322	F	F	F
0.6671611611272414	0.3327435024167358	0.2124532032647530	T	T	T
0.6666706163169209	0.5333294306830751	0.0442400867929322	F	F	F
0.6647571073490616	0.5322249289940170	0.2130079547066399	T	T	T
0.6666706163169209	0.7333294186830770	0.0442400867929322	F	F	F
0.6686849261990195	0.7342926972756175	0.2119457099755888	T	T	T
0.6666706163169209	0.9333294066830788	0.0442400867929322	F	F	F
0.6646830098335501	0.9324279591205921	0.2130266583604014	T	T	T
0.8666706043169228	0.1333294096830784	0.0442400867929322	F	F	F
0.8668754671146519	0.1330885246873821	0.2128223504514835	T	T	T
0.8666706043169228	0.3333294126830779	0.0442400867929322	F	F	F
0.8655424490508388	0.3327446618378463	0.2124377474661675	T	T	T
0.8666706043169228	0.5333294306830751	0.0442400867929322	F	F	F
0.8668158742579827	0.5337259558071143	0.2128069922057728	T	T	T
0.8666706043169228	0.7333294186830770	0.0442400867929322	F	F	F
0.8665889084812041	0.7322404242136819	0.2125658545636606	T	T	T
0.8666706043169228	0.9333294066830788	0.0442400867929322	F	F	F
0.8666442615970676	0.9344398495157991	0.2126117449844962	T	T	T
0.1333271469929400	0.0666728560070595	0.1234950372465988	F	F	F

0.1335544587654920	0.0671692397173527	0.2913270699588199	T	T	T
0.1333271469929400	0.2666728440070614	0.1234950372465988	F	F	F
0.1332428348027258	0.2667413686623957	0.2918048175239840	T	T	T
0.1333271469929400	0.4666728620070586	0.1234950372465988	F	F	F
0.1325315429555408	0.4662900153370454	0.2939290806272317	T	T	T
0.1333271469929400	0.6666728790070593	0.1234950372465988	F	F	F
0.1332564985495720	0.6665652261097537	0.2918011723166447	T	T	T
0.1333271469929400	0.8666728670070611	0.1234950372465988	F	F	F
0.1335675286751800	0.8663469344820921	0.2913625851219257	T	T	T
0.3333271499929396	0.0666728560070595	0.1234950372465988	F	F	F
0.3331873461874646	0.0666371592619802	0.2923881948209271	T	T	T
0.3333271499929396	0.2666728440070614	0.1234950372465988	F	F	F
0.3334195064344737	0.2667134165718212	0.2917983625603340	T	T	T
0.3333271499929396	0.4666728620070586	0.1234950372465988	F	F	F
0.3323893344312246	0.4649170834169477	0.2906313356392559	T	T	T
0.3333271499929396	0.6666728790070593	0.1234950372465988	F	F	F
0.3324274489895909	0.6675202275322696	0.2906525900524168	T	T	T
0.3333271499929396	0.8666728670070611	0.1234950372465988	F	F	F
0.3333849298181288	0.8667005149923021	0.2918045167854791	T	T	T
0.5333271679929368	0.0666728560070595	0.1234950372465988	F	F	F
0.5337211037039888	0.0667109822880053	0.2917602623122048	T	T	T
0.5333271679929368	0.2666728440070614	0.1234950372465988	F	F	F
0.5337182810768192	0.2670142405558195	0.2917715383568284	T	T	T
0.5333271679929368	0.4666728620070586	0.1234950372465988	F	F	F
0.5337107724781518	0.4662242095904987	0.2938851108213414	T	T	T
0.5333271679929368	0.6666728790070593	0.1234950372465988	F	F	F
0.5350353122316494	0.6675621109539903	0.2906333248845753	T	T	T
0.5333271679929368	0.8666728670070611	0.1234950372465988	F	F	F
0.5336570187831121	0.8674032115576416	0.2939183730558801	T	T	T
0.7333271559929386	0.0666728560070595	0.1234950372465988	F	F	F
0.7328966560535257	0.0666596607522237	0.2917443364176730	T	T	T
0.7333271559929386	0.2666728440070614	0.1234950372465988	F	F	F
0.7333024417529321	0.2665977448455245	0.2923130096803643	T	T	T
0.7333271559929386	0.4666728620070586	0.1234950372465988	F	F	F
0.7329096823028711	0.4661790026651022	0.2917712215806736	T	T	T
0.7333271559929386	0.6666728790070593	0.1234950372465988	F	F	F
0.7332341310386034	0.6665105024273182	0.2918015899207210	T	T	T
0.7333271559929386	0.8666728670070611	0.1234950372465988	F	F	F
0.7332132902144725	0.8666681896103611	0.2918105851432510	T	T	T
0.9333271439929405	0.0666728560070595	0.1234950372465988	F	F	F
0.9333162961809949	0.0666356609186873	0.2924475077398668	T	T	T
0.9333271439929405	0.2666728440070614	0.1234950372465988	F	F	F
0.9332801338663859	0.2670610636632189	0.2917566432210019	T	T	T
0.9333271439929405	0.4666728620070586	0.1234950372465988	F	F	F
0.9332354293435325	0.4662036946228924	0.2917531510989647	T	T	T
0.9333271439929405	0.6666728790070593	0.1234950372465988	F	F	F

0.9332924098046801 0.6667386144404273 0.2923794893919742 T T T
0.9333271439929405 0.8666728670070611 0.1234950372465988 F F F
0.9327682142414065 0.8663634732648259 0.2913375212784449 T T T

Zr(001) Subsurface Octahedral with Sn on Surface

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16.2854995727999992 0.0000000000000000 0.0000000000000000
-8.1427497863999996 14.1036563433000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.2423000335999994
T Sn Zr
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Direct
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0.3311930756566989 0.4623462882770096 0.3070960162840001 T T T
0.0666705933169212 0.1333294096830784 0.0442400867929322 F F F
0.0666044466636553 0.1315364234969257 0.2120481075002769 T T T
0.0666705933169212 0.3333294126830779 0.0442400867929322 F F F
0.0629922954981772 0.3315762827737344 0.2117725502405307 T T T
0.0666705933169212 0.5333294306830751 0.0442400867929322 F F F
0.0696828023640236 0.5345106742493833 0.2121451498415532 T T T
0.0666705933169212 0.7333294186830770 0.0442400867929322 F F F
0.0649637105694057 0.7307386386906878 0.2132746862822509 T T T
0.0666705933169212 0.9333294066830788 0.0442400867929322 F F F
0.0663916362305643 0.9327815409380656 0.2131625199727602 T T T
0.2666705813169230 0.1333294096830784 0.0442400867929322 F F F
0.2649365086867759 0.1315688729619730 0.2120607285590016 T T T
0.2666705813169230 0.3333294126830779 0.0442400867929322 F F F
0.2678697754611666 0.3355925570160950 0.2123574753038721 T T T
0.2666705813169230 0.5333294306830751 0.0442400867929322 F F F
0.2649536253222182 0.5279033926761223 0.2119534644065052 T T T
0.2666705813169230 0.7333294186830770 0.0442400867929322 F F F
0.2639187695818566 0.7341361917358369 0.2119879504980079 T T T
0.2666705813169230 0.9333294066830788 0.0442400867929322 F F F
0.2662060526899879 0.9332585591912995 0.2117429979599261 T T T
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0.4677854922011750 0.1329955224775028 0.2132910303267136 T T T
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0.4666705993169202 0.5333294306830751 0.0442400867929322 F F F
0.4630693813587900 0.5279649783469940 0.2119535071023128 T T T
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0.4709606673637471 0.7419288099928260 0.2118435706980738 T T T
0.4666705993169202 0.9333294066830788 0.0442400867929322 F F F

0.4681479448177093	0.9350561566452059	0.2129153434685218	T	T	T
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0.6664480288446657	0.1330418893728887	0.2125067373096490	T	T	T
0.6666706163169209	0.3333294126830779	0.0442400867929322	F	F	F
0.6665591518135634	0.3322405879348106	0.2131352472780109	T	T	T
0.6666706163169209	0.5333294306830751	0.0442400867929322	F	F	F
0.6648986991387484	0.5344782060631413	0.2121470388557286	T	T	T
0.6666706163169209	0.7333294186830770	0.0442400867929322	F	F	F
0.6701890953206280	0.7341389385332366	0.2119998787159530	T	T	T
0.6666706163169209	0.9333294066830788	0.0442400867929322	F	F	F
0.6668077101381881	0.9350813212357996	0.2129093597094800	T	T	T
0.8666706043169228	0.1333294096830784	0.0442400867929322	F	F	F
0.8650953916788279	0.1330269143796191	0.2132872748871612	T	T	T
0.8666706043169228	0.3333294126830779	0.0442400867929322	F	F	F
0.8656781625980369	0.3322318014260582	0.2131443743653926	T	T	T
0.8666706043169228	0.5333294306830751	0.0442400867929322	F	F	F
0.8670011035479613	0.5340114849044701	0.2117760949167300	T	T	T
0.8666706043169228	0.7333294186830770	0.0442400867929322	F	F	F
0.8657209752591976	0.7307110408350647	0.2132853700729529	T	T	T
0.8666706043169228	0.9333294066830788	0.0442400867929322	F	F	F
0.8669787624895400	0.9332730500341772	0.2117275457535626	T	T	T
0.1333271469929400	0.0666728560070595	0.1234950372465988	F	F	F
0.1342377735314342	0.0685667018851971	0.2921948636699055	T	T	T
0.1333271469929400	0.2666728440070614	0.1234950372465988	F	F	F
0.1369155558020217	0.2709701949282424	0.2901305207948219	T	T	T
0.1333271469929400	0.4666728620070586	0.1234950372465988	F	F	F
0.1379752838832519	0.4644429474557674	0.2909860678628208	T	T	T
0.1333271469929400	0.6666728790070593	0.1234950372465988	F	F	F
0.1344626683442506	0.6647640618547285	0.2927607771346863	T	T	T
0.1333271469929400	0.8666728670070611	0.1234950372465988	F	F	F
0.1345897031449864	0.8660891743966904	0.2914304764601037	T	T	T
0.3333271499929396	0.0666728560070595	0.1234950372465988	F	F	F
0.3329186847622642	0.0661824113431847	0.2914127678585391	T	T	T
0.3333271499929396	0.2666728440070614	0.1234950372465988	F	F	F
0.3340909432900654	0.2709479750492649	0.2901756647128803	T	T	T
0.3333271499929396	0.4666728620070586	0.1234950372465988	F	F	F
0.3333271499929396	0.6666728790070593	0.1234950372465988	F	F	F
0.3322031849354861	0.6619536309363672	0.2895733866387118	T	T	T
0.3333271499929396	0.8666728670070611	0.1234950372465988	F	F	F
0.3334274921431903	0.8666667962994150	0.2914015820898723	T	T	T
0.5333271679929368	0.0666728560070595	0.1234950372465988	F	F	F
0.5342955142439011	0.0671666876190437	0.2928186947632520	T	T	T
0.5333271679929368	0.2666728440070614	0.1234950372465988	F	F	F
0.5324828801152338	0.2669003900054311	0.2930068590558332	T	T	T
0.5333271679929368	0.4666728620070586	0.1234950372465988	F	F	F
0.5265190313646863	0.4644543629502986	0.2909877917365276	T	T	T

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0.9333271439929405 0.2666728440070614 0.1234950372465988 F F F
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0.9344349544779451 0.4675764502025284 0.2908465315380580 T T T
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0.9321029627092196 0.6642053371749935 0.2925916912075862 T T T
0.9333271439929405 0.8666728670070611 0.1234950372465988 F F F
0.9313974223978032 0.8660707667354609 0.2913943859825233 T T T

Zr(001) Subsurface Octahedral with Sn on Subsurface

0001_4_layer
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16.2854995727999992 0.0000000000000000 0.0000000000000000
-8.1427497863999996 14.1036563433000008 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.2423000335999994
T Sn Zr
1 1 99
Direct
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0.4676513653809891 0.5323265452749653 0.2056786297768483
0.0668190915295733 0.1336444605408088 0.0448426319589858
0.0622046761469205 0.1321594715490909 0.2119555498688745
0.0688117933598403 0.3348582217942703 0.0453260826969680
0.0704689687908837 0.3365085597210224 0.2132203397024681
0.0668134727572074 0.5321352619526136 0.0448878226078340
0.0670148379660940 0.5325508217751197 0.2114228529105128
0.0672753972048448 0.7344912997669505 0.0421092114109568
0.0675524969499203 0.7366454380505436 0.2121331122049579

0.0670724888722998 0.9328954595932439 0.0437258781623962
0.0691516975988851 0.9307998973794395 0.2121845365138299
0.2650032657007594 0.1306515177979528 0.0432747862583610
0.2726790633746438 0.1396610669611464 0.2120731593147769
0.2677300664637601 0.3341295497801441 0.0436626026804338
0.2682530349739465 0.3307756737432894 0.2127266076833947
0.2671592014262784 0.5335916347254730 0.0448733244233896
0.2661781687186867 0.5349131251620750 0.2161937596132926
0.2648931384768220 0.7350617188604862 0.0430531464136698
0.2670910554370674 0.7328564202061438 0.2114201673263509
0.2654880496242553 0.9327028145331997 0.0421150960670583
0.2633465431133076 0.9324785398994022 0.2121357860035950
0.4673468229881280 0.1334865233335394 0.0449676209426707
0.4671121091805512 0.1294815858779953 0.2117889635831197
0.4673193971319082 0.3330310250796842 0.0436050040919823
0.4639192947250981 0.3366383674714890 0.2135308301508747
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0.4663401419017946 0.7327421534858030 0.0448971892614271
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0.4678135199252068 0.9331484095205526 0.0449079397370184
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0.8666240873737944 0.1332862427864720 0.2130254066501081
0.8669038491587217 0.3320151369745627 0.0441324457926445
0.8678830841482955 0.3330724409290056 0.2124963452494960
0.8664945408684674 0.5326157857896336 0.0449900375243280
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0.8603326752400622 0.7272813519303659 0.2120750696292719
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0.1337406220600303 0.0676745504152689 0.2889880289761886
0.1362149122306783 0.2671805667510873 0.1237495098311345
0.1360024020063073 0.2659800453461040 0.2912516525449128
0.1365254224667349 0.4686620398417837 0.1251415571545158

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0.1315653884814022 0.6678696121178599 0.1224936297082562
0.1313589295797372 0.6651269358040007 0.2901604366066760
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0.1338920574740835 0.8660847852030902 0.2937633282600773
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0.3320218028396109 0.2632826725543147 0.1221327633062191
0.3345627057814381 0.2674698404387013 0.2960477326657418
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0.3409019628153261 0.4655415829460640 0.2900550398787752
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0.3320474450030052 0.8683556742017785 0.1224993380503739
0.3348237702991673 0.8685860296902460 0.2901425509908542
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0.9322874401284064 0.8662159725780091 0.2889985138072838

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