Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supplement for Mechanistic insights into rubidium ion adsorption at the quartz (101) surface from quantum chemical metadynamics‡

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Table of Contents

Table S1: Simulation time depth

Pristine	Trajectory per walker (from HILLS)	Total sampling	Defect	Trajectory per walker (from HILLS)	Total sampling
Geminal_234	318	12.72	Geminal_234	446	17.84
Vacancy_234	327	13.08	Vacancy_234	442	17.68
Vicinal_217	327	13.08	Vicinal_217	444	17.76
Vicinal_222	386	15.44	Vicinal_222	424	16.96
Vicinal_223	402	16.08	Vicinal_223	451	18.04
Vicinal_238	381	15.24	Vicinal_238	425	17.00

The total trajectory per walker in picoseconds and the total sampling in nanoseconds. The total sampling is across 40 walkers.

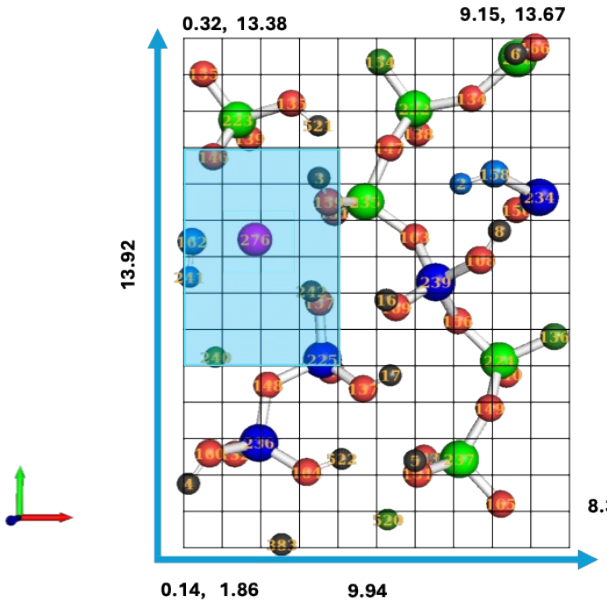
Table S2: Surface distances

Pristine	Surface, Å	Defect	Surface, Å
Geminal 234	7.537	Geminal 234	7.537
Vacancy 234	7.537	Vacancy 234	7.343
Vicinal 217	7.537	Vicinal 217	7.543
Vicinal 222	7.537	Vicinal 222	7.343
Vicinal 223	7.537	Vicinal 223	7.443
Vicinal 238	7.537	Vicinal 238	7.443

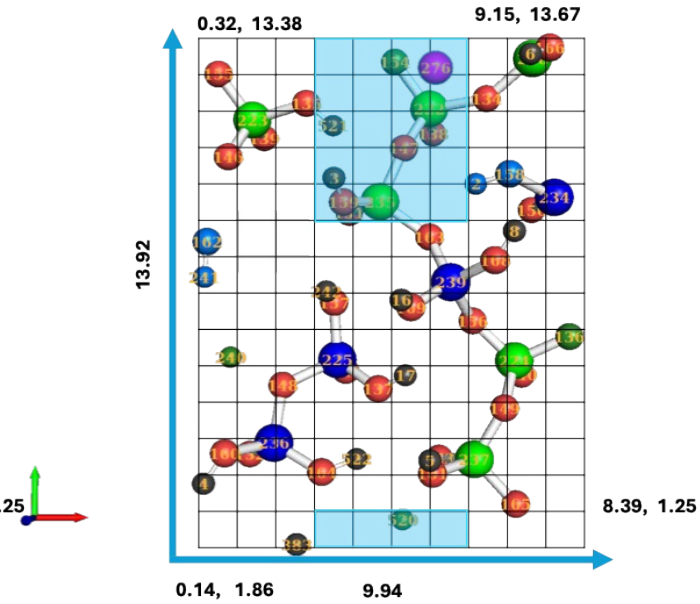
Surface distances were calculated using the z-projection of the electron density plot generated with VMD 1.9.4 at 0.1 Å-resolution, and identifying the silanol silicon peak, averaging the electron density over nanosecond trajectories for each system.

Simulation conditions

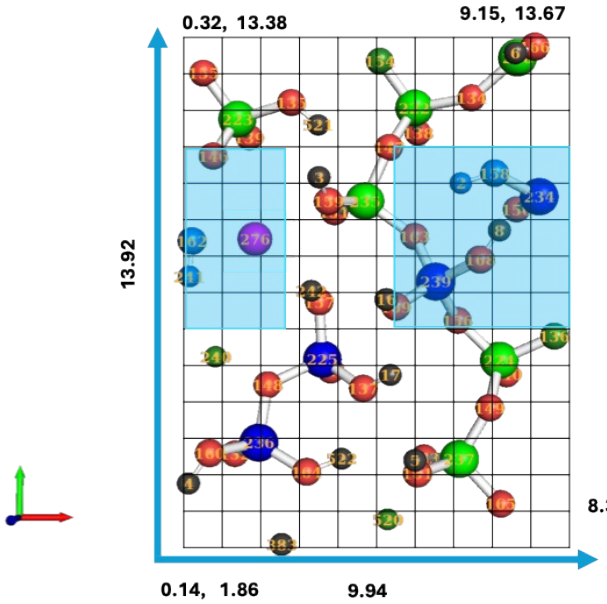
Vacancy 234



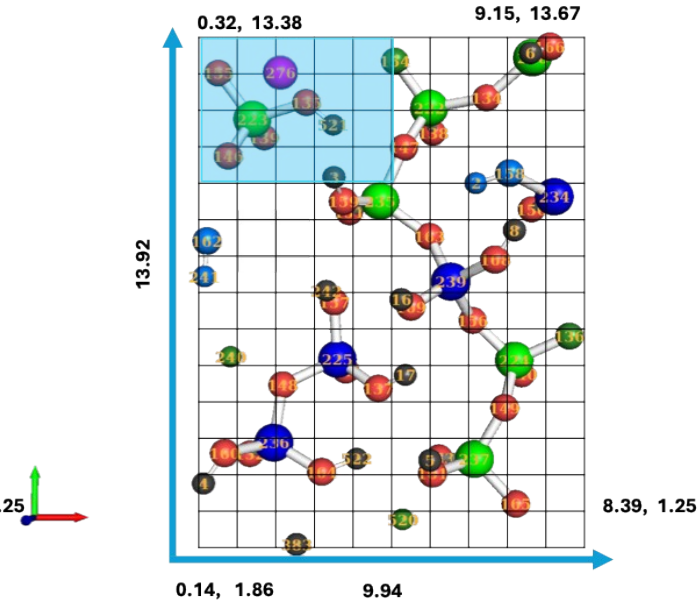
Vicinal 222



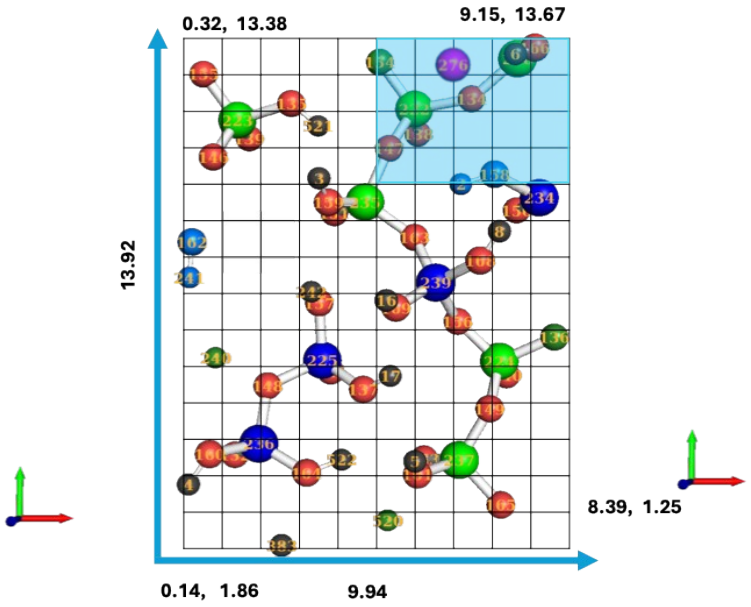
Geminal 234



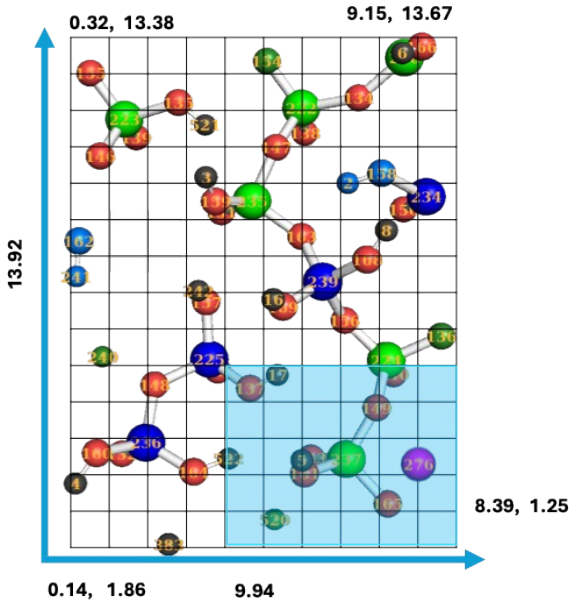
Vicinal 223



Vicinal 238



Vicinal 217



Collective variable definitions

Coordination CV

The coordination collective variable is for the silanol oxygen to all water oxygens (Si-o=O:Ow). The silanol oxygen is the hydroxyl oxygen of the silanol (for example, the surface equivalent to silicon 234 for the geminal 234 simulations). The water oxygens are all solvent oxygens, identified using OpenPymol. The coordination definition is such that s_{ij} is 1 if the contact between atoms i in group A and j in group B is formed, and zero otherwise. This follows the default switching function s_{ij}, implemented in PLUMED.[1, 2]

$$\sum_{i \in A} \sum_{i \in B} s_{ij}$$

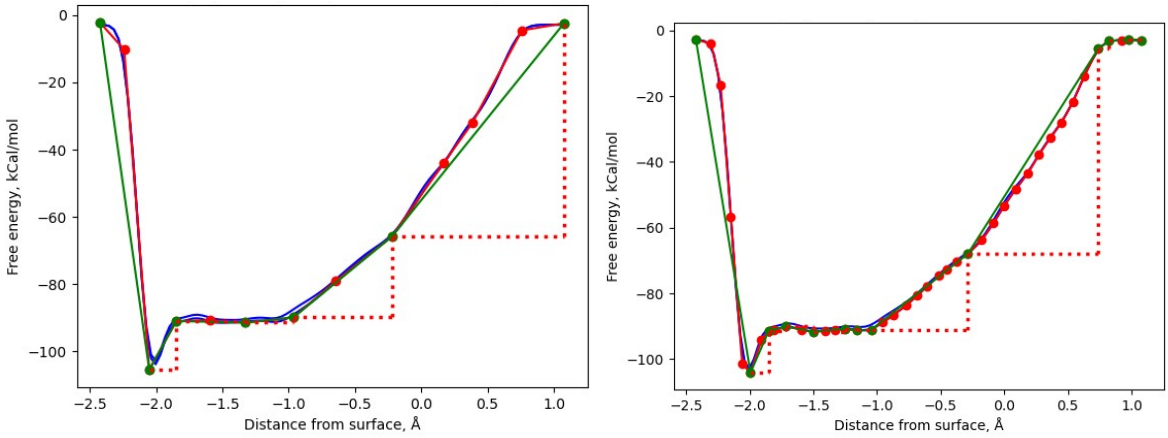
$$s_{ij} = \frac{1 - \left(\frac{r_{ij} - d_0}{r_0}\right)^n}{1 - \left(\frac{r_{ij} - d_0}{r_0}\right)^m}$$

Rb^+ Distance to Surface CV

The distance collective variable is the z-component of a Euclidean distance between a frozen silicon atom in the lowermost quartz layer, and the Rb+, which in post-processing is corrected

with the distance between the frozen silicon atom and the surface, which is assessed by electron particle density plots from VMD (see also, Figure S1).

Illustration: Ramer-Douglas-Peucker approach



12 line segments in the regression fit, RDP epsilon 0.46, 40 line segments in the regression fit, RDP epsilon 0.16. Here using an unconverged FES (free energy in kcal·mol^{-1}) from the Pristine Vacancy 234 system.

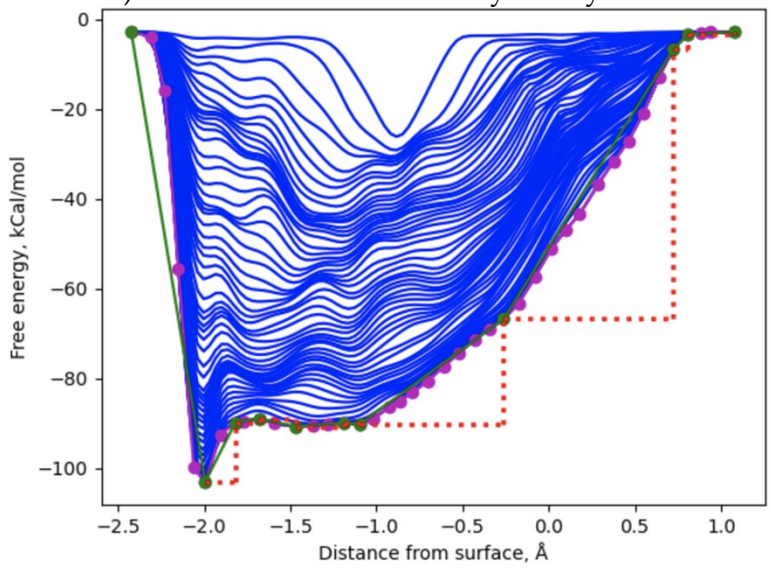
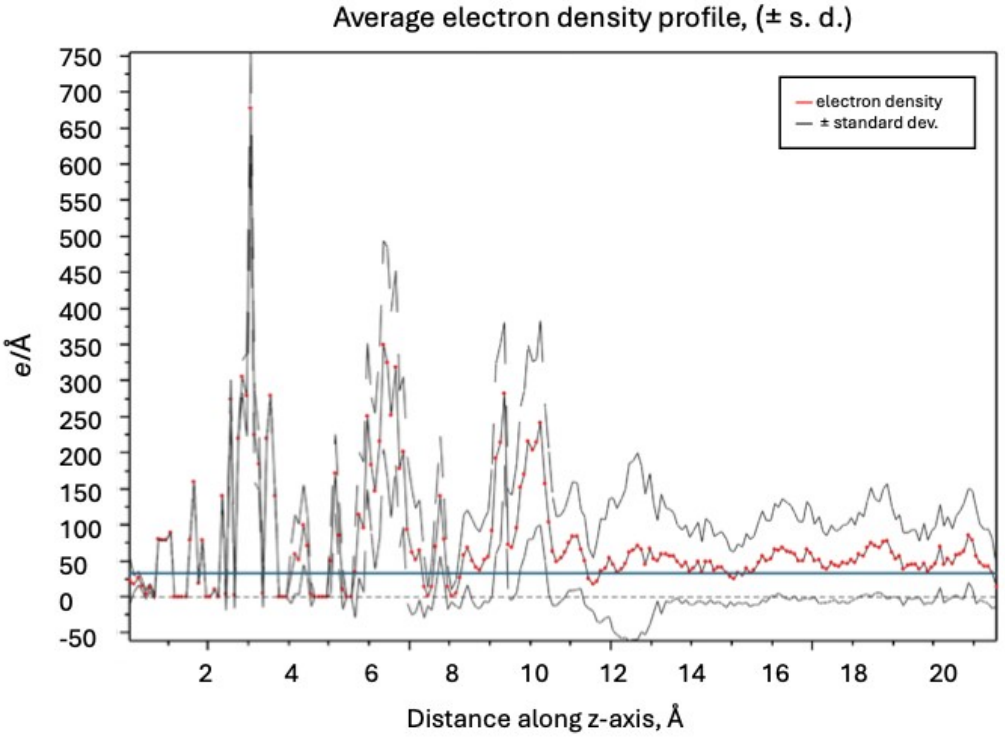
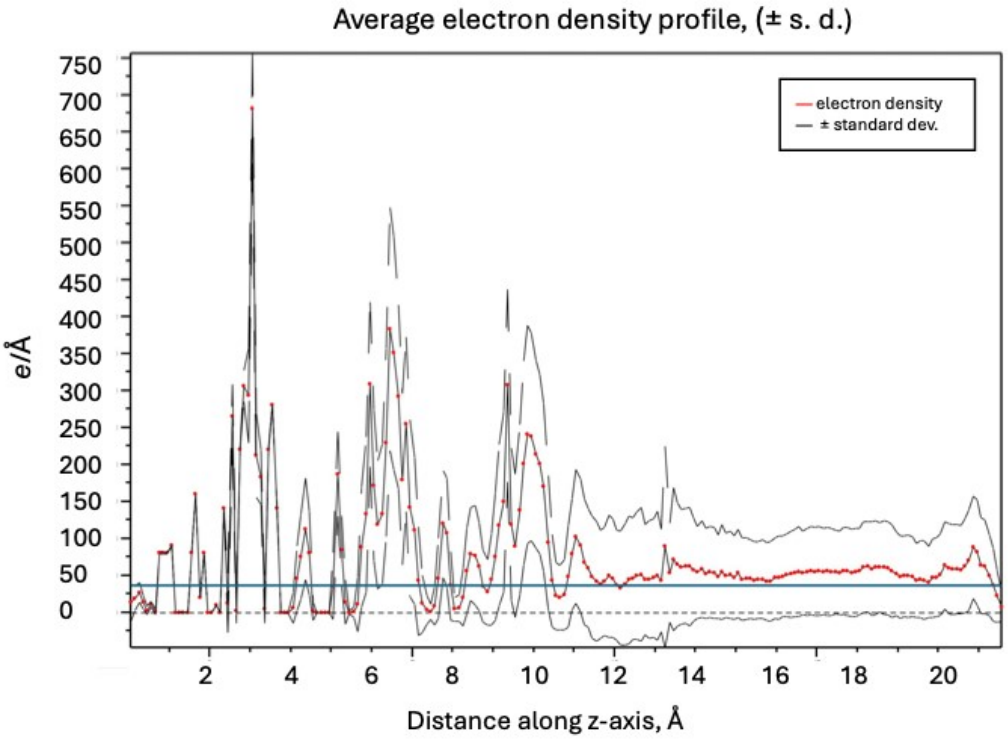


Figure S1: Convergence in the water structure

A



B



C

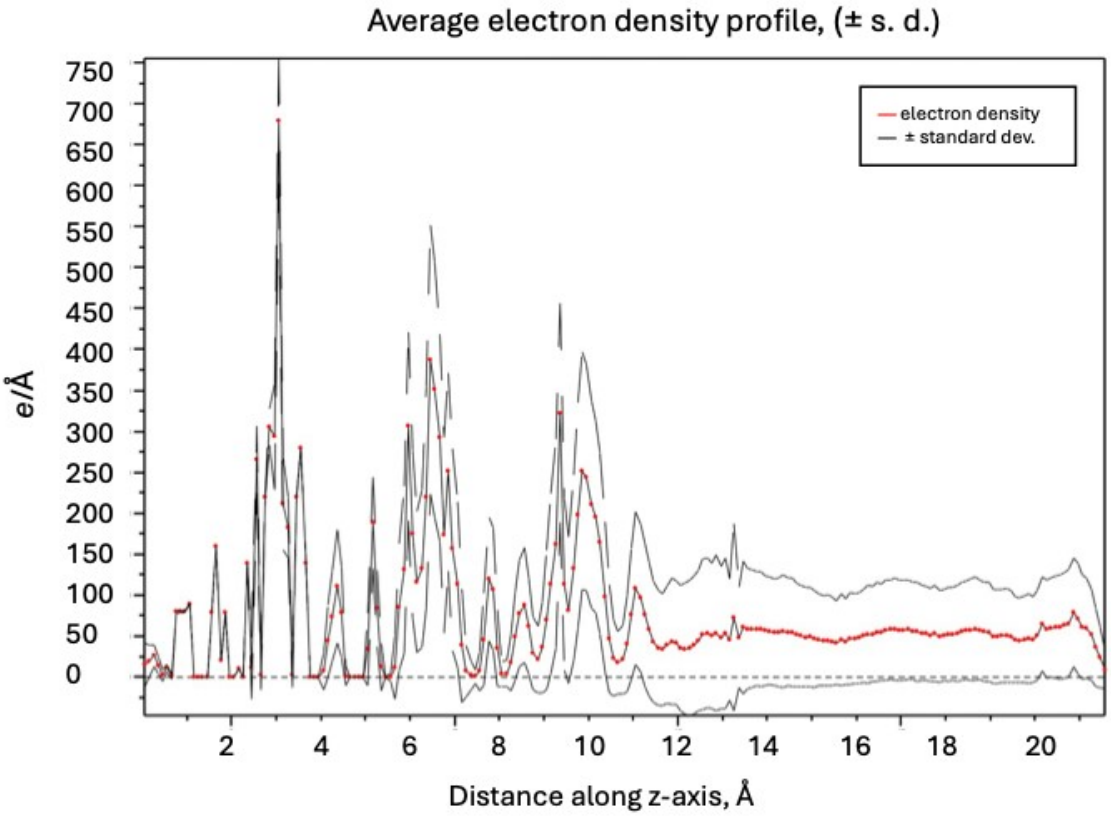
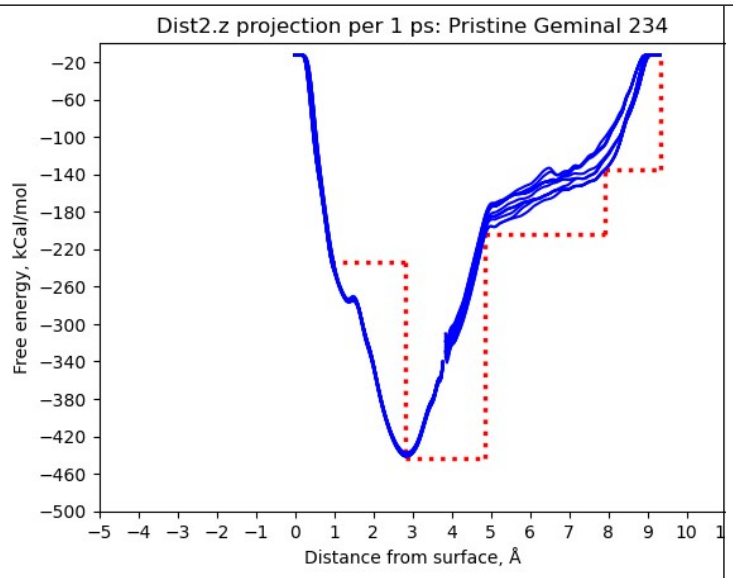


Figure S1: z-projections of particle density plots (VMD), intensity vs. z-coordinate in Å, for the equilibrated system, after an additional 30 ps for 50 ps total, and after 290 ps. Comparing particle density plots for the initial equilibrated structure (A), structure after 50 ps (B), and structure after 290 ps (C), convergence in the water structure was obtained after a further 30 ps of equilibration from the initial equilibration, for a total of 50 ps. The blue line in A and B is at the electron density of bulk water, (33 *e*/Å), corresponding to 0.33 *e*/Å^3.

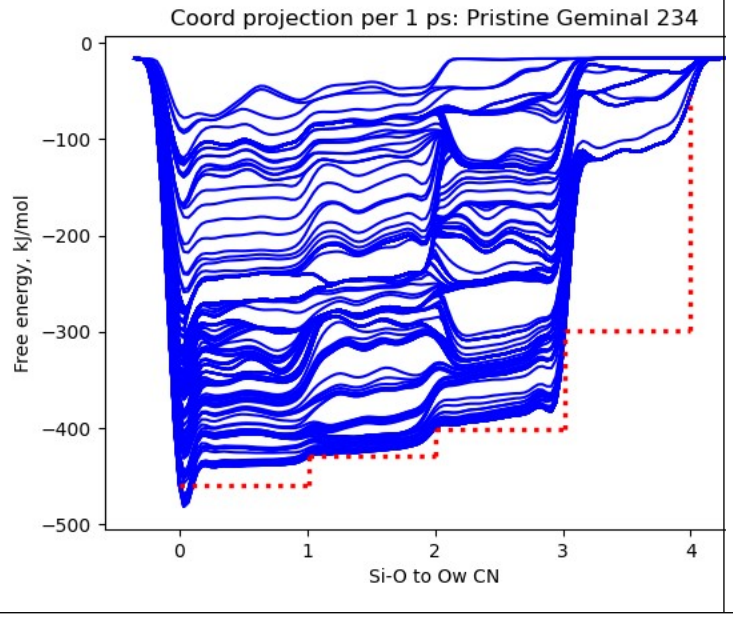
Table S3: FES projections along the CVs

At minimally 12 ns (40 walkers at 318 ps, Pristine Geminal 234)
Maximally 18 ns (40 walkers at 451 ps, Defect Vicinal_223).

Pristine Geminal 234

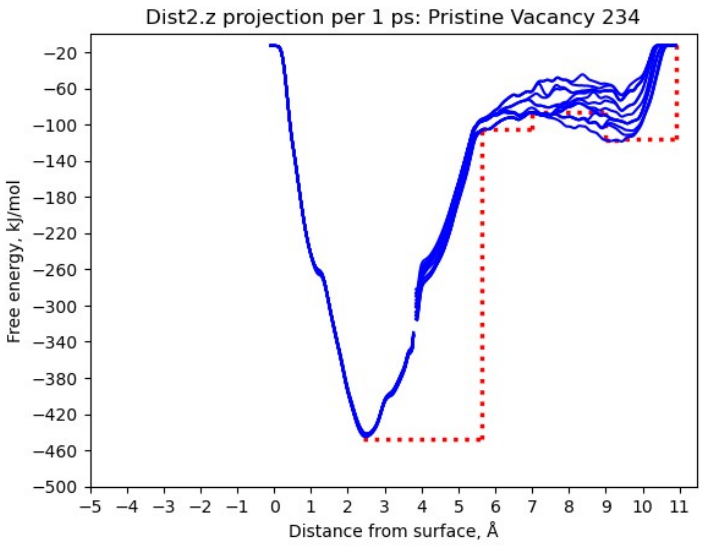


	Distance	Energy change
0	2.82	-209.38
1	4.85	239.64
2	7.93	68.69
3	9.32	122.91

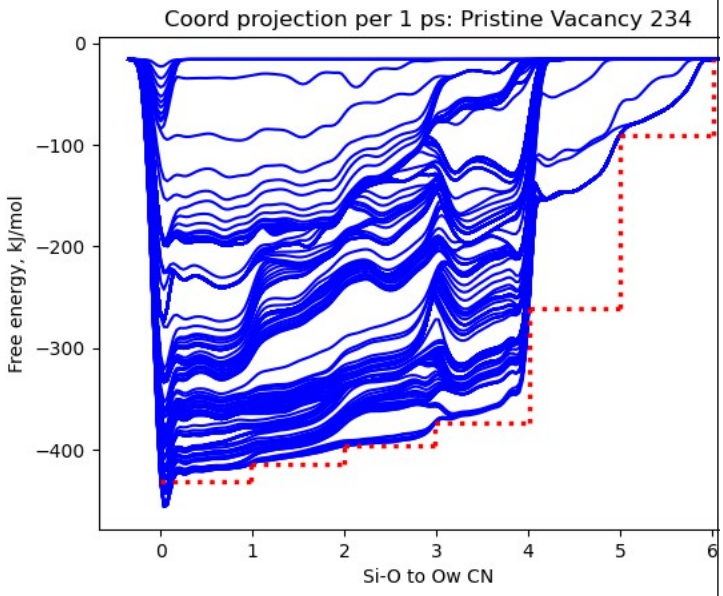


	Coordination	Energy change
0	1.02	30.01
1	2.00	27.95
2	3.02	101.90
3	4.00	244.87

Pristine: Vacancy_234

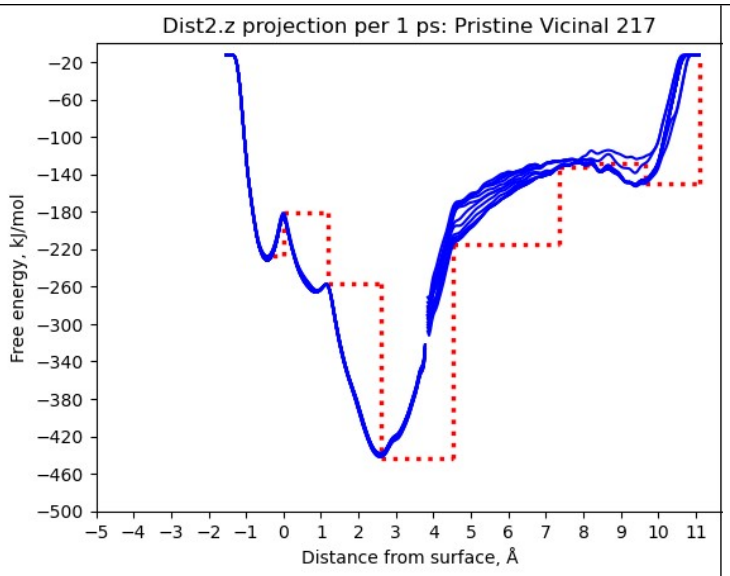


	Distance	Energy change
0	5.63	341.26
1	6.99	19.32
2	8.97	-31.11
3	9.22	-0.70
4	9.51	1.48
5	10.91	105.40

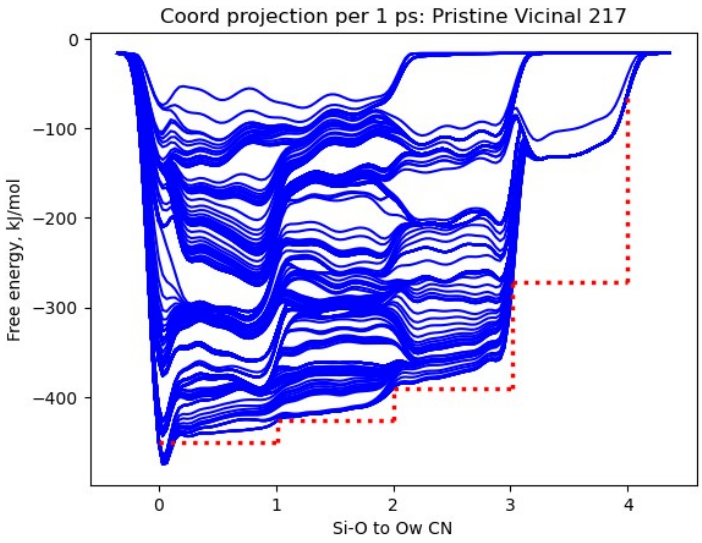


	Coordination	Energy change
0	0.98	17.87
1	2.00	17.91
2	2.99	22.13
3	4.01	112.84
4	4.99	170.34
5	6.01	74.83

Pristine Vicinal 217

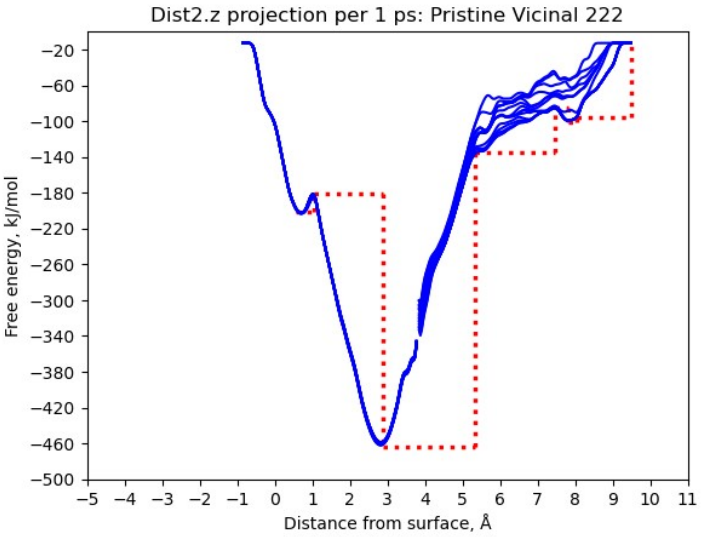


	Distance	Energy change
0	-0.00	45.40
1	1.19	-75.13
2	2.59	-187.30
3	4.52	229.11
4	7.36	81.92
5	8.10	4.20
6	9.66	-21.96
7	11.09	136.06

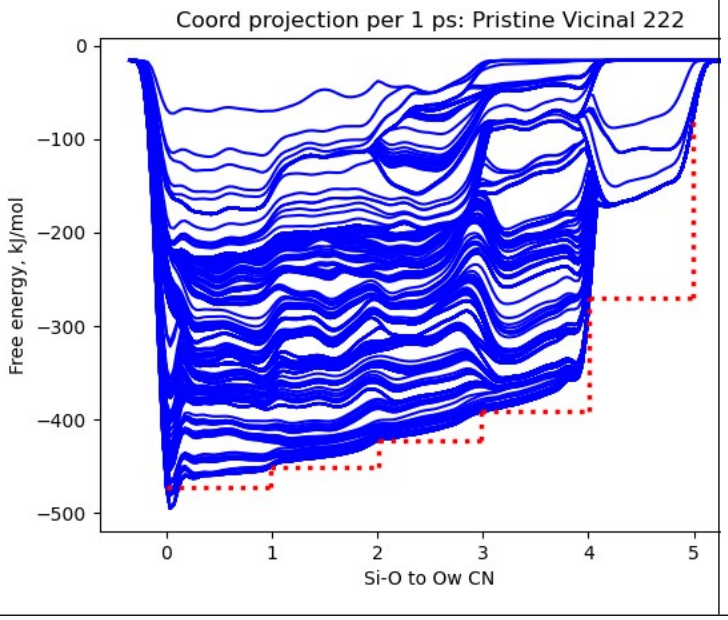


	Coordination	Energy change
0	1.02	24.23
1	2.00	35.64
2	3.02	119.18
3	4.00	209.13

Pristine Vicinal 222

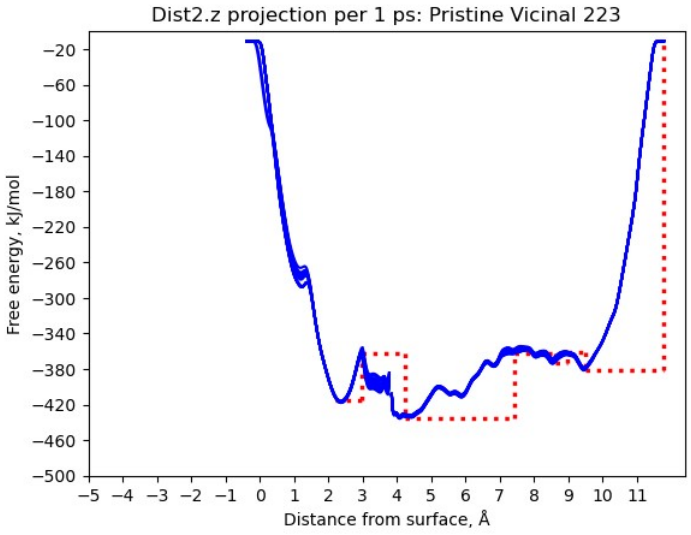


	Distance	Energy change
0	1.05	20.08
1	2.87	-283.21
2	5.32	329.10
3	7.48	50.09
4	7.81	-15.82
5	8.05	4.69
6	9.48	84.65

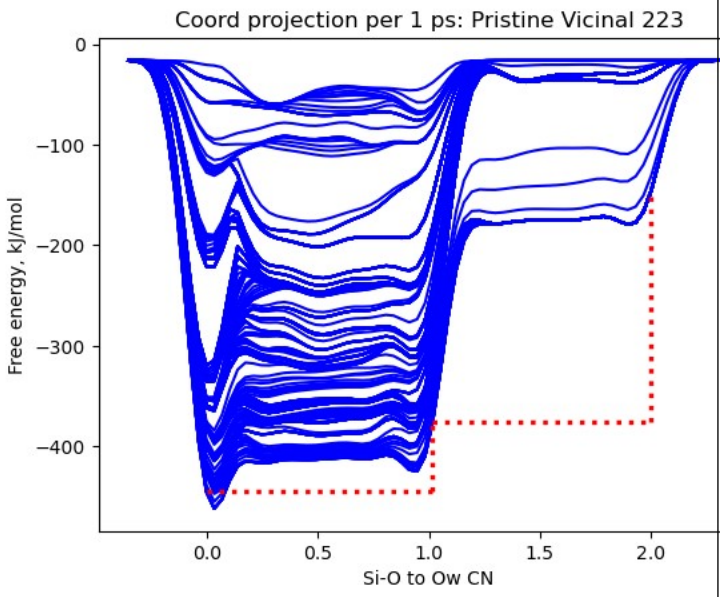


	Coordination	Energy change
0	0.98	21.96
1	2.00	28.35
2	2.99	31.03
3	4.01	120.80
4	5.00	193.85

Pristine Vicinal 223

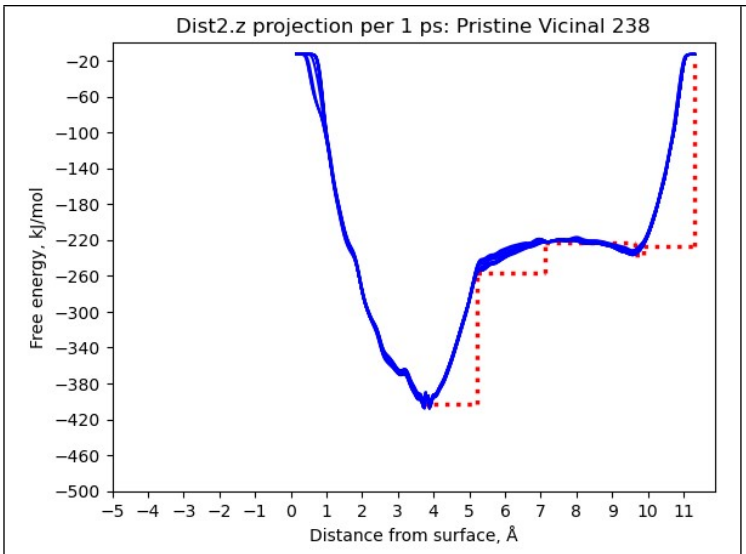


	Distance	Energy change
0	2.96	53.23
1	4.23	-73.00
2	7.44	73.32
3	8.62	-11.43
4	8.98	12.68
5	9.50	-21.15
6	11.78	368.69

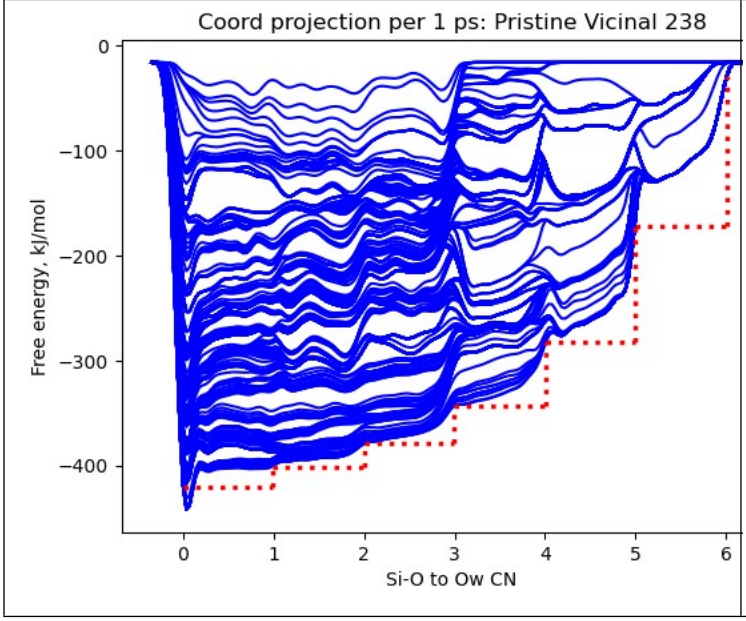


	Coordination	Energy change
0	1.02	70.12
1	2.00	229.92

Pristine Vicinal 238

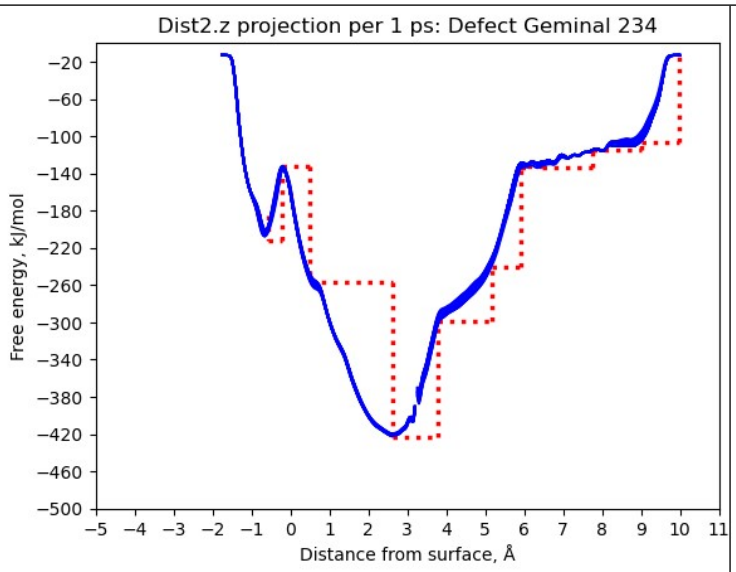


	Distance	Energy change
0	5.21	146.06
1	7.13	33.74
2	9.64	-14.18
3	9.86	9.53
4	11.31	211.80

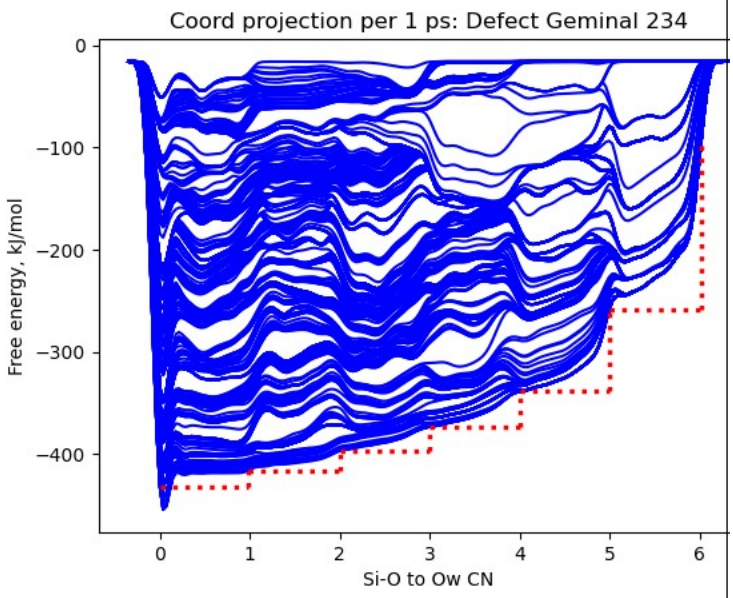


	Coordination	Energy change
0	0.98	19.11
1	2.00	22.02
2	2.99	35.20
3	4.01	61.07
4	4.99	111.06
5	6.01	142.75

Defect Geminal 234

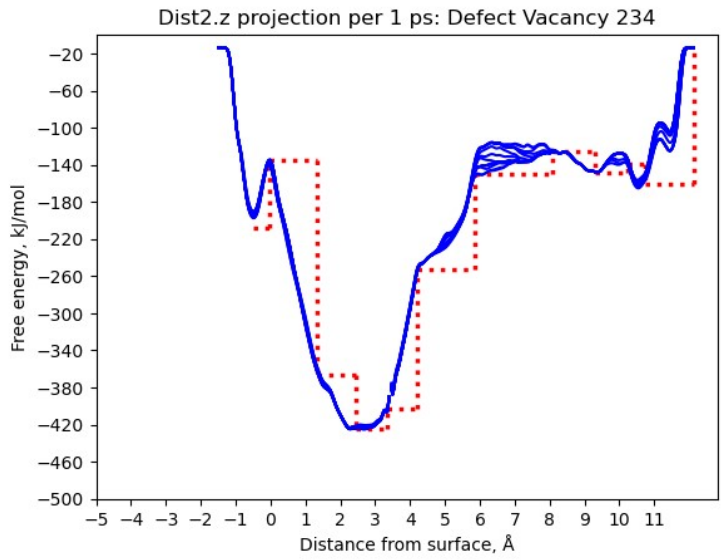


	Distance	Energy change
0	-0.57	-26.00
1	-0.20	79.81
2	0.50	-125.35
3	2.62	-165.61
4	3.80	123.96
5	5.18	58.48
6	5.91	106.55
7	6.07	1.45
8	6.48	-0.63
9	7.74	17.98
10	9.02	8.28
11	9.99	91.55

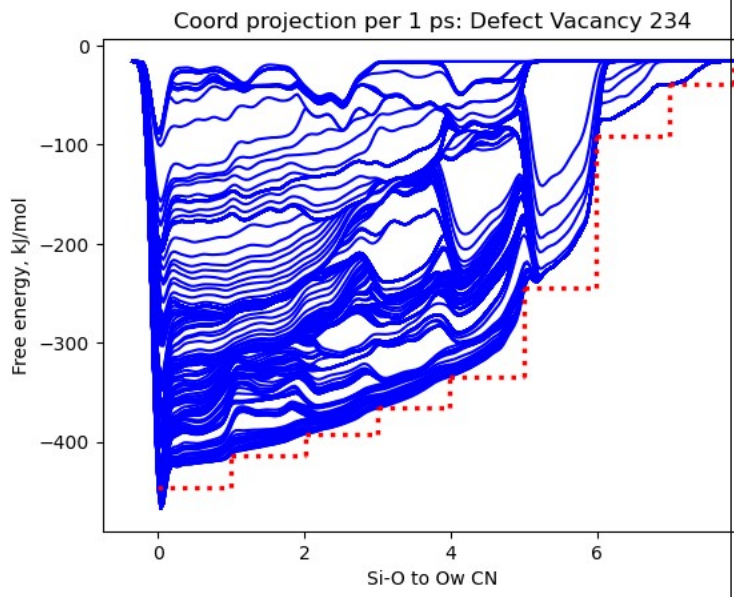


	Coordination	Energy change
0	0.98	16.28
1	2.00	19.27
2	2.99	23.22
3	4.01	34.65
4	5.00	80.51
5	6.02	162.17

Defect Vacancy 234

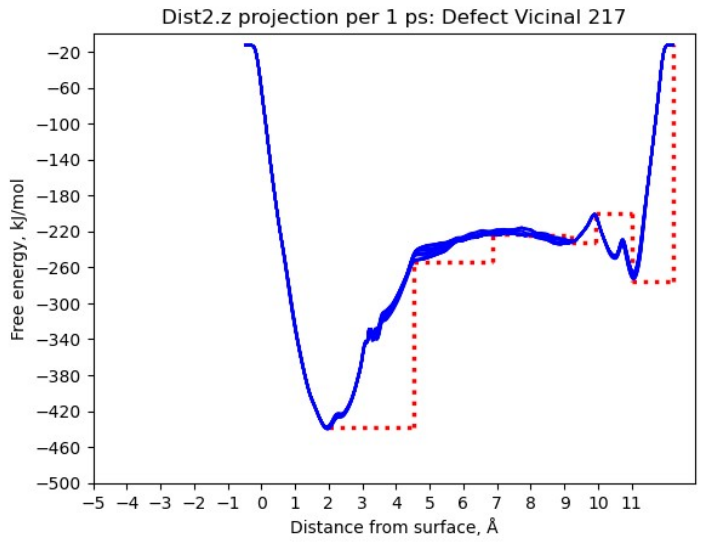


	Distance	Energy change
0	-0.04	73.08
1	1.33	-232.10
2	2.46	-58.44
3	3.33	22.39
4	4.20	150.09
5	5.85	102.25
6	8.07	24.33
7	9.30	-22.86
8	10.24	10.20
9	10.73	-21.86
10	12.12	145.62

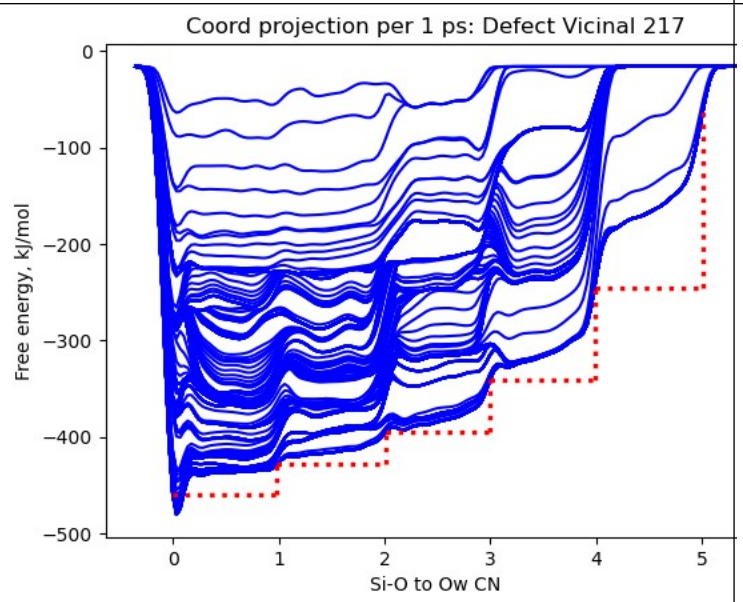


	Coordination	Energy change
0	0.99	32.57
1	2.01	21.64
2	3.00	25.81
3	3.99	31.83
4	5.01	88.91
5	6.00	153.22
6	6.99	52.64
7	7.87	23.11

Defect Vicinal 217

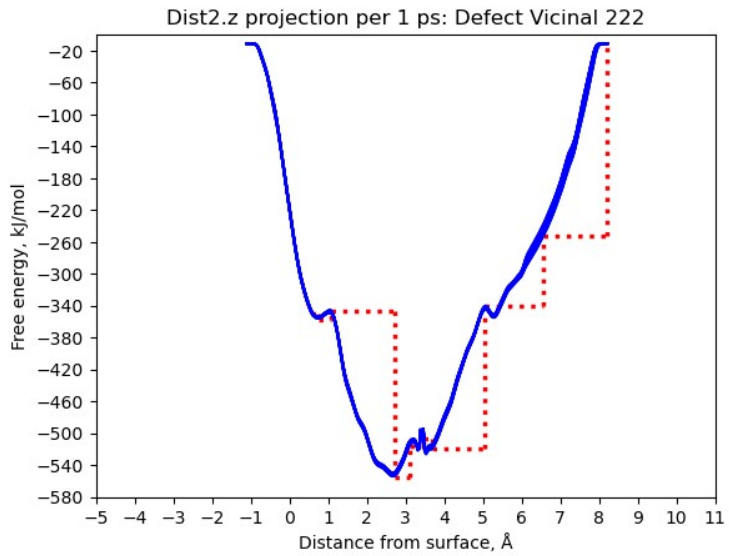


	Distance	Energy change
0	4.51	184.51
1	6.85	30.27
2	7.22	0.91
3	7.91	-1.62
4	9.23	-8.57
5	9.93	32.65
6	11.01	-75.32
7	12.23	263.45

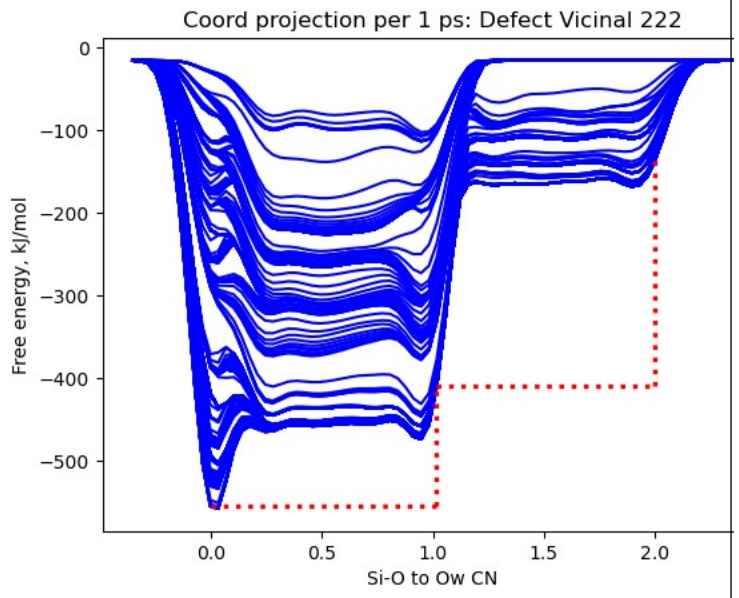


	Coordination	Energy change
0	0.99	31.53
1	2.01	33.00
2	3.00	54.18
3	3.98	96.01
4	5.01	182.38

Defect Vicinal 222

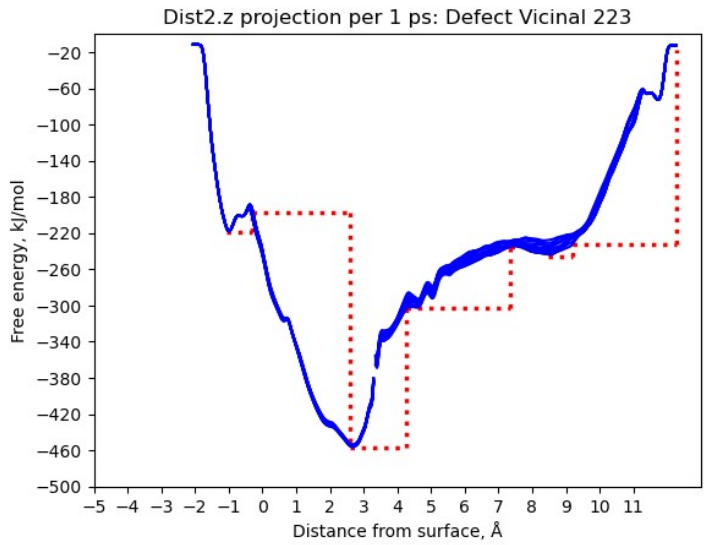


	Distance	Energy change
0	0.77	-6.89
1	1.07	10.28
2	2.72	-208.75
3	3.11	38.79
4	3.46	10.51
5	3.70	-13.91
6	5.05	178.83
7	6.58	89.12
8	8.22	242.28

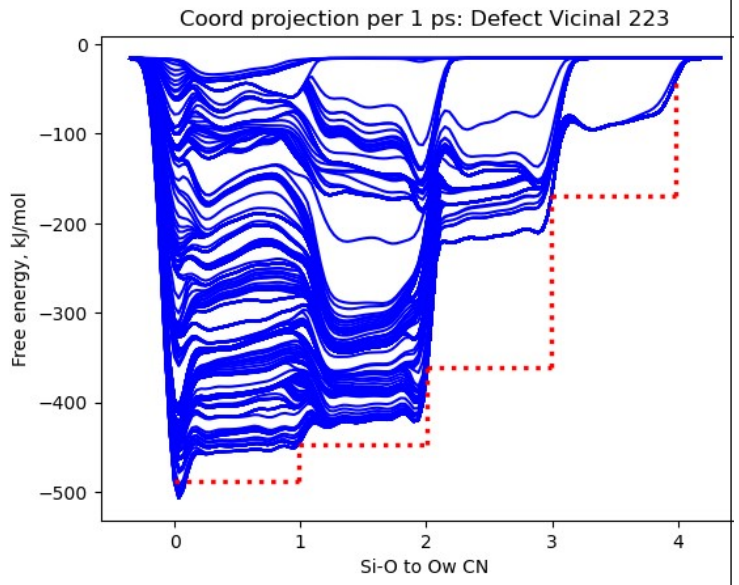


	Coordination	Energy change
0	1.02	145.42
1	2.00	273.65

Defect Vicinal 223

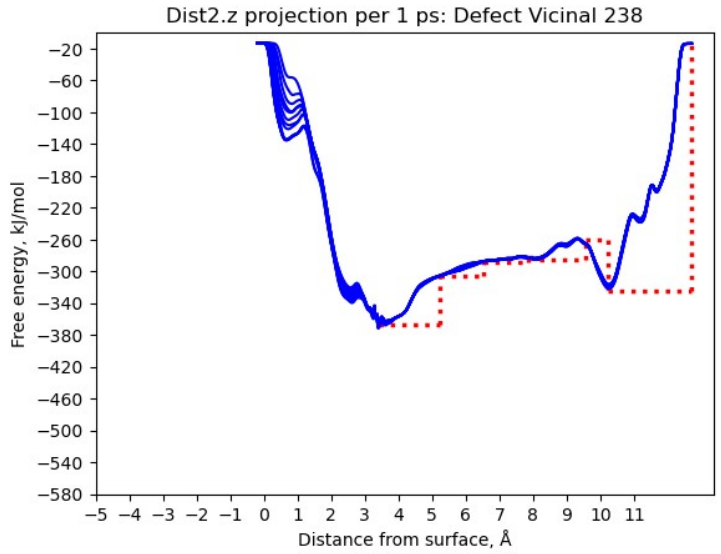


	Distance	Energy change
0	-0.32	21.19
1	2.60	-259.44
2	4.27	154.13
3	7.36	68.08
4	8.47	-10.88
5	9.21	12.80
6	12.27	215.28

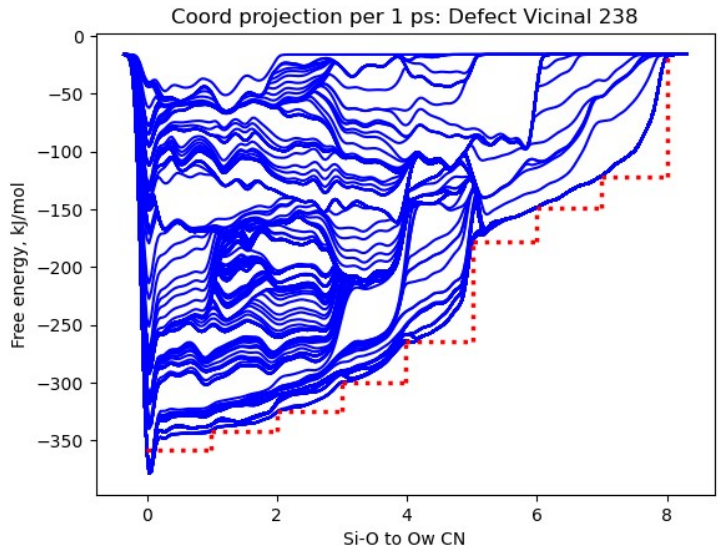


	Coordination	Energy change
0	0.99	41.26
1	2.01	86.03
2	3.00	191.57
3	3.98	129.07

Defect Vicinal 238



	Distance	Energy change
0	5.22	61.25
1	6.51	17.72
2	7.87	5.10
3	8.18	-2.94
4	9.55	25.43
5	10.24	-64.01
6	12.70	310.27



	Coordination	Energy change
0	0.99	16.58
1	2.01	16.72
2	3.00	25.55
3	3.99	34.67
4	5.01	86.51
5	6.00	29.84
6	6.99	26.87
7	8.01	104.84

Tables S4 and S5: Equilibrium constants

For comparison across sites, we use the approach from Lee *et al.*,[3] to solve for the standard-state intrinsic cation adsorption constant, K_M°, as $\Delta G_{ads,M}^\circ = -RTlnK_M^\circ$. As could be expected from the relative energetics, both outer-sphere and inner-sphere adsorption occurs readily, K_M° >> 0, whereas incorporation is endergonic, K_M° ≈ 0, and expected to be rarely observed at equilibrium.

Pristine cases

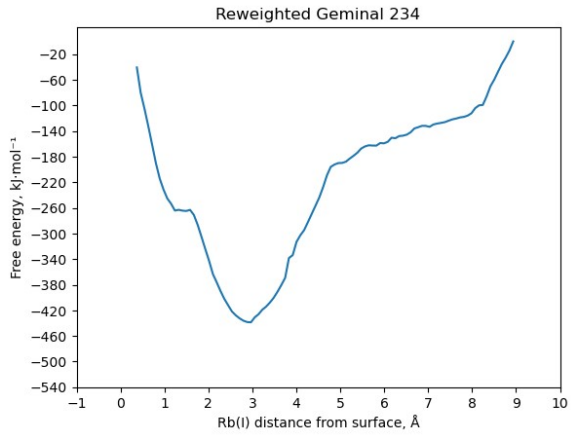
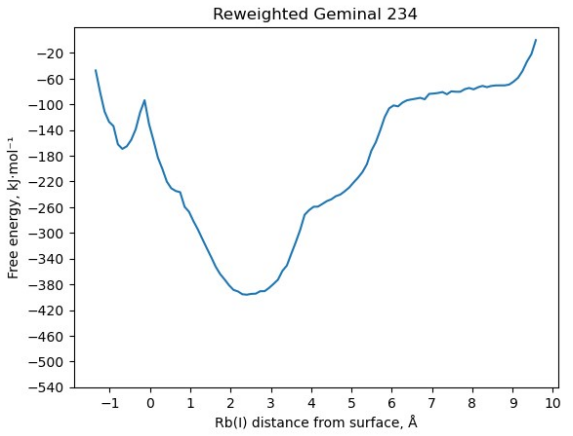
Geminal_234	
Inner sphere	9.52E+41
Outer-sphere	1.09E+12
Vacancy_234	
Inner-sphere	2.35E+36
Outer-sphere	2.66E+23
Vicinal 217	
Incorporated	6.96E-14
Inner-sphere	1.38E+40
Outer-sphere	2.23E+14
Vicinal 222	
Incorporated	3.03E-04
Inner-sphere	4.56E+57
Outer-sphere	5.99E+08
Vicinal 223	
Unconverged	
Vicinal 238	
Inner-sphere	3.95E+25
Outer-sphere	8.02E+05

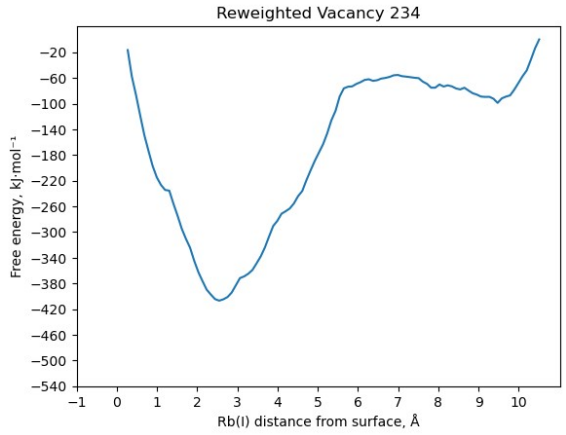
Defect cases

Geminal_234	
Incorporated	2.78E-05
Inner-sphere	8.25E+31
Outer-sphere	4.75E+18
Vacancy_234	
Incorporated	1.56E-13
Inner-sphere	1.67E+30
Outer-sphere	8.38E+17
Vicinal 217	
Inner-sphere	2.11E+32
Outer-sphere	2.04E+05
Vicinal 222	
Incorporated	6.18E-02
Inner-sphere	3.38E+37
Outer-sphere	4.08E+15
Vicinal 223	
Incorporated	1.93E-04
Inner-sphere	9.97E+26
Outer-sphere	8.54E+11
Vicinal 238	
Unconverged	

Table S6: Reweighted FES projections

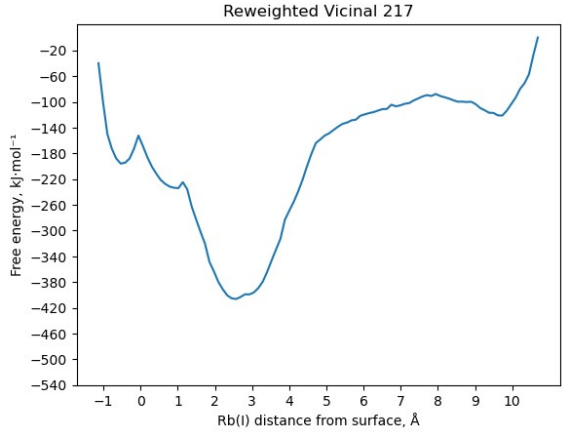
When the Rb^+ z-coordinate exceeded half the unit cell height, the measure in PLUMED flipped to the silicon atom on the z-periodic reflection. As a result, there was oversampling at the half cell-height (11.350 Å for the pristine surface, and 10.772 Å for the defect surface). This produced spikes in the FES at those values (Unweighted FES, SI). To address this, the reweighting protocol from Invernizzi and Parrinello[4] was followed. First, the COLVARS were partitioned into two COLVARS files: one with Rb^+ z-coordinates up to the half-cell parameter distance, and one including the half cell-height and beyond. The cell height was subtracted from each value in the latter so that the measure was consistent between both sets. Then, the FES was projected separately for each COLVARS file. Then, the two FES were plotted on the ranges for the COLVARS, with the first up to the half cell-height, and the second from the half-cell height to the remaining sampled range. This was sufficient alone to give a corrected FES, since the difference in bin widths where the two plots overlapped was only 0.05 Å. Nonetheless, histogram reweighting was also performed to gauge any changes in the FES. The weights were calculated from the metadynamics bias, using the same k_bT factor (2.49) as the simulations and with simple exponential reweighting, as $e^{\frac{bias}{kbt}}$.[5] The FES was then projected from histogram binning with 100 bins, using the calculated weights.

Pristine	Defect
Geminal 234	Geminal 234
	
Vacancy 234	Vacancy 234

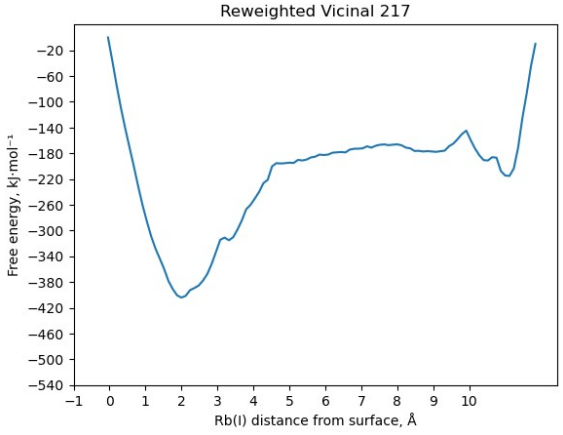


Vicinal 217

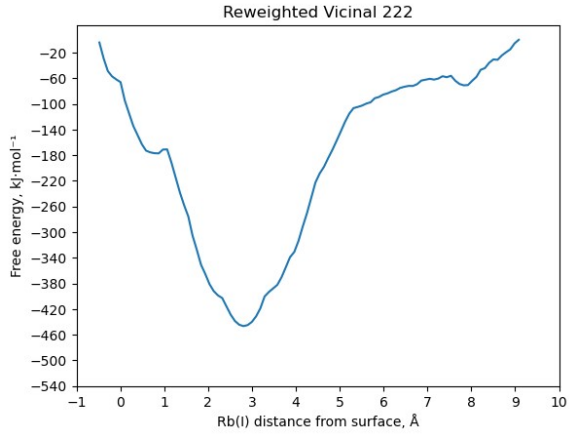
Vicinal 217



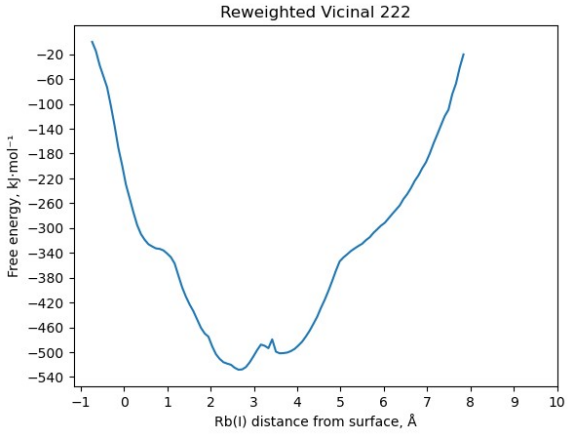
Vicinal 222



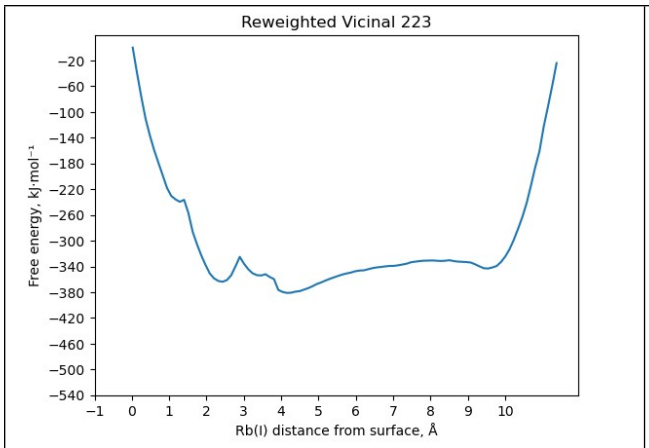
Vicinal 222

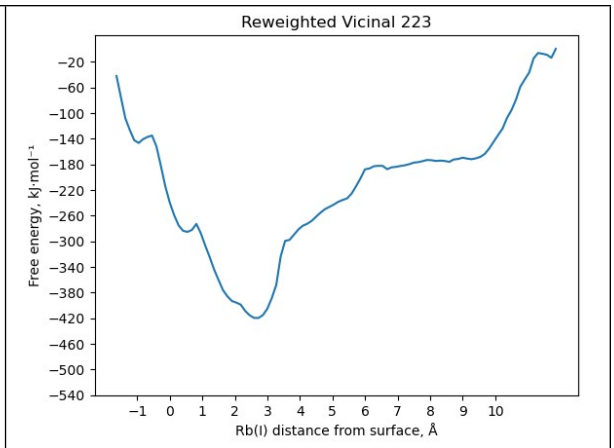


Vicinal 223



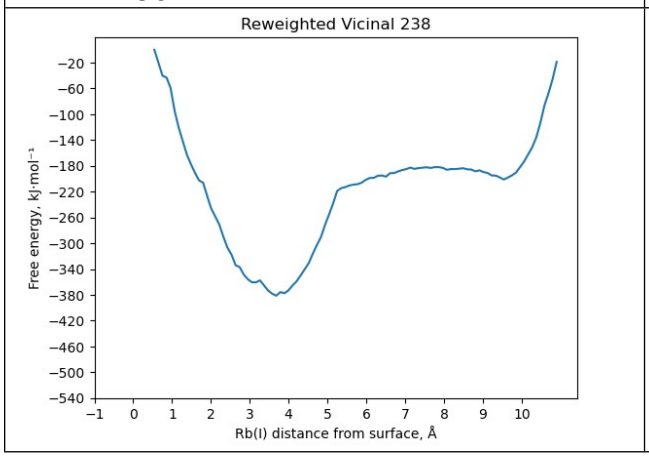
Vicinal 223





Vicinal 238

Vicinal 238



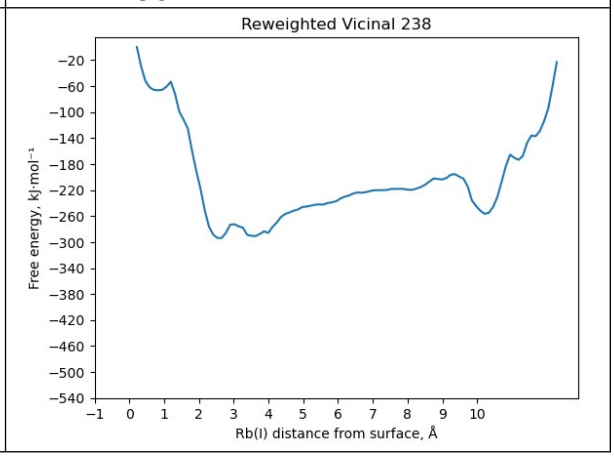
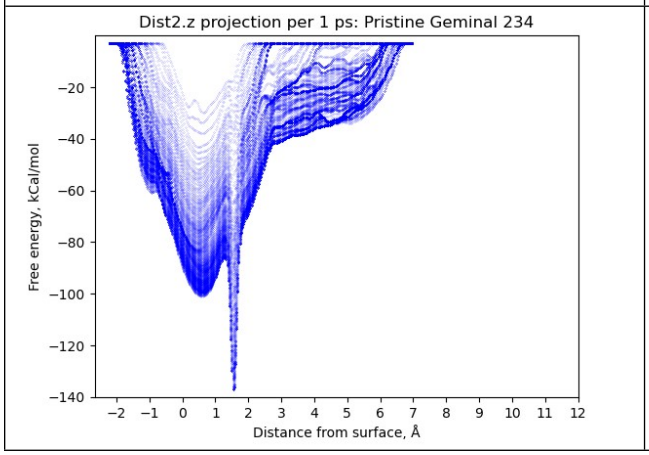
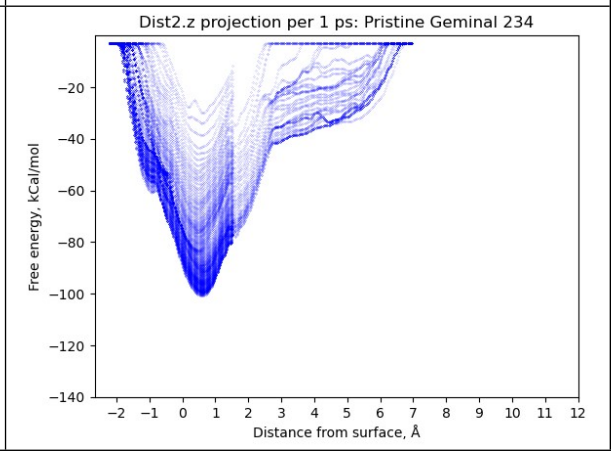


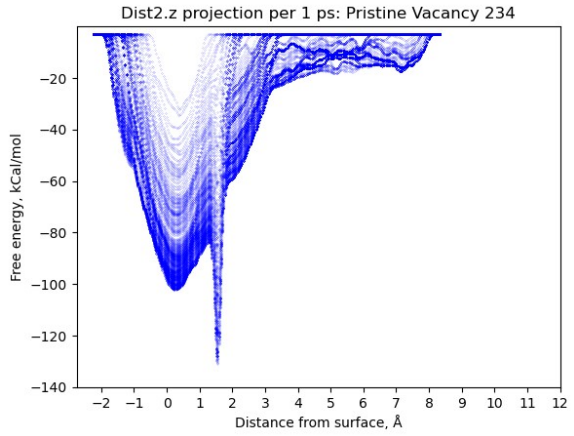
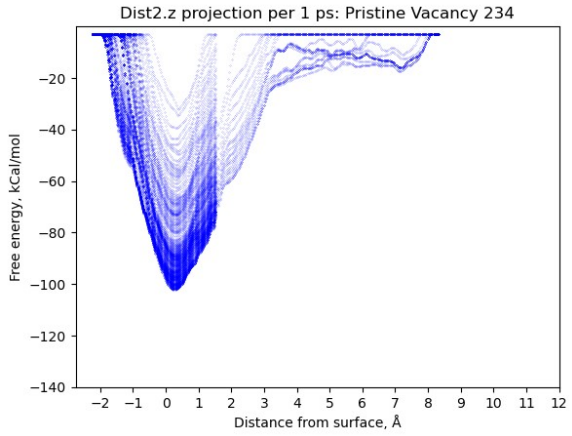
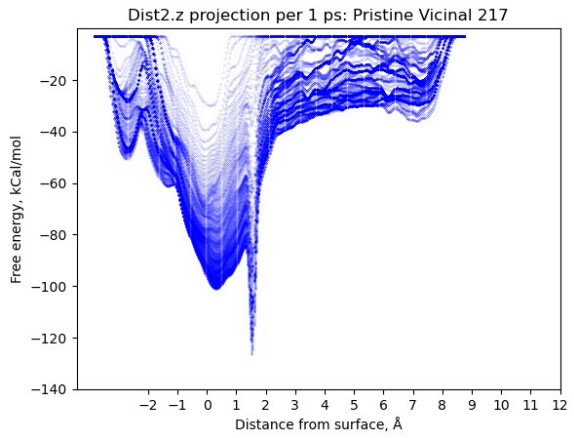
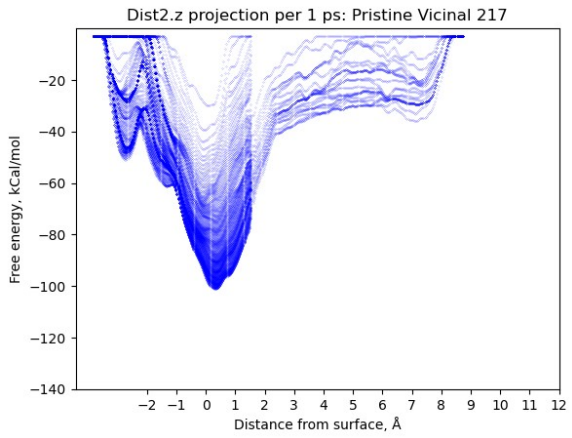
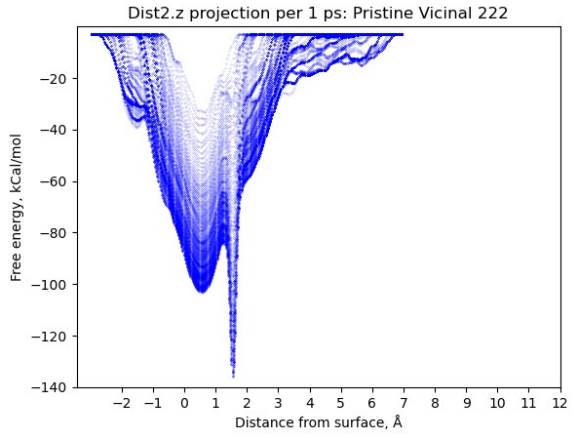
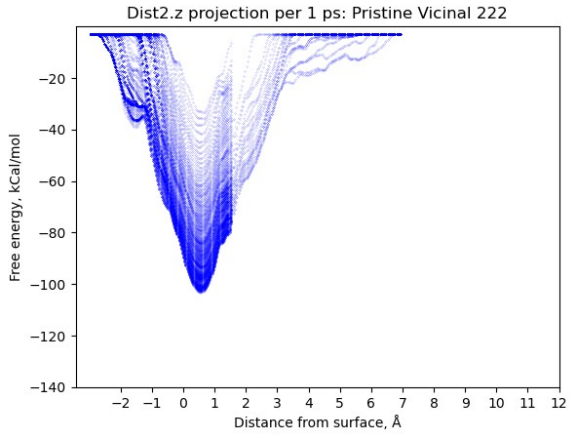
Table S7: Half cell-height oversampling and correction

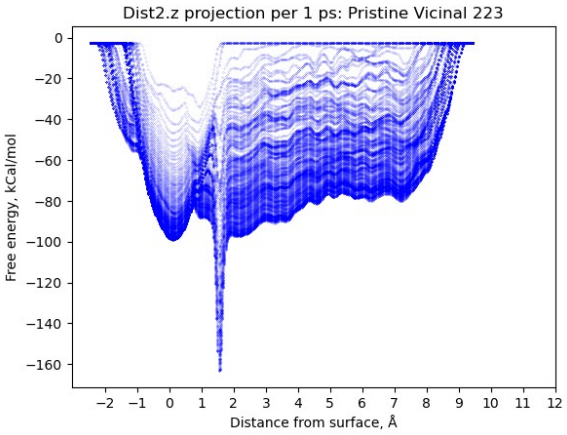
Minimally 9.48 ns of sampling (pristine Geminal 234). This shows the evolution of the FES over the last quarter of the trajectory, when compared with the Projected FES section.
Pristine cases

Original	Range-based projection
Geminal 234	Geminal 234

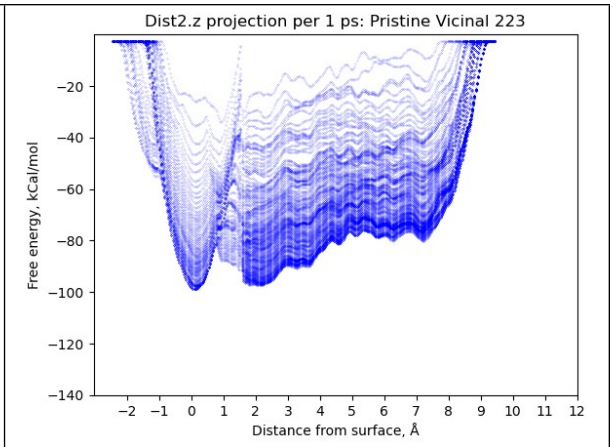




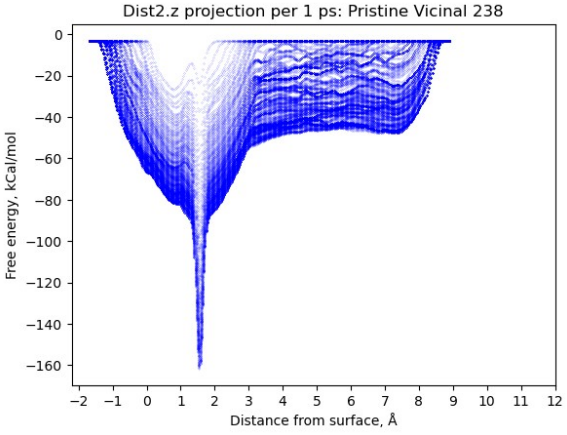
Vacancy 234	Vacancy 234
	
Vicinal 217	Vicinal 217
	
Vicinal 222	Vicinal 222
	
Vicinal 223	Vicinal 223

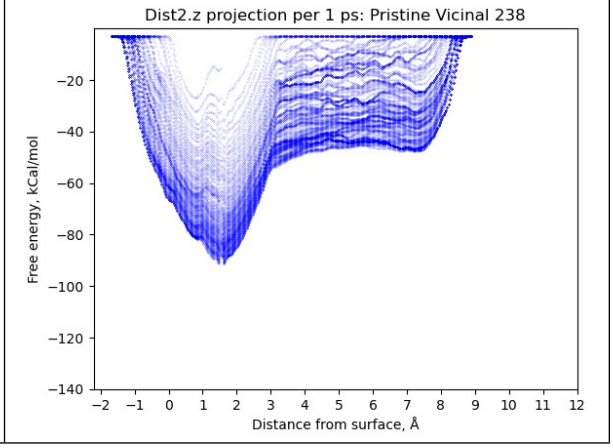


Vicinal 238

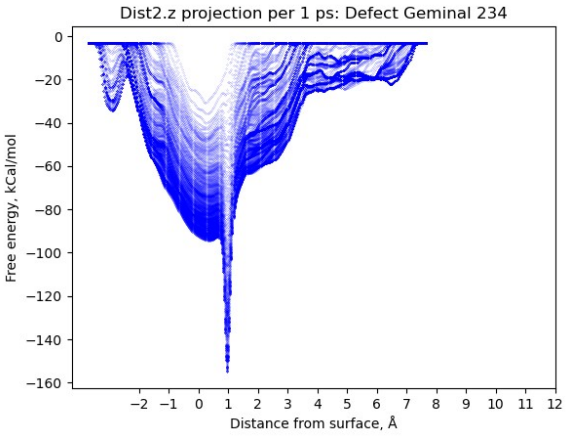
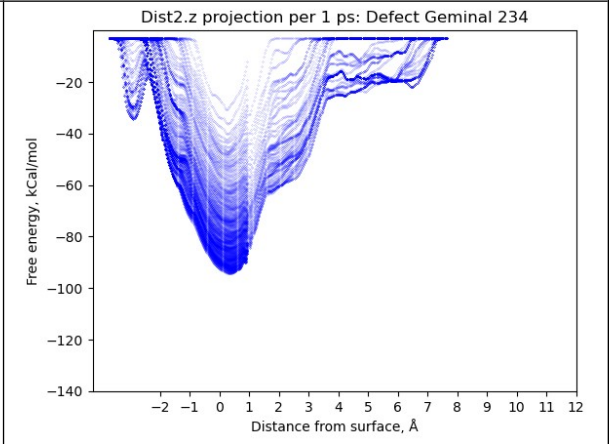


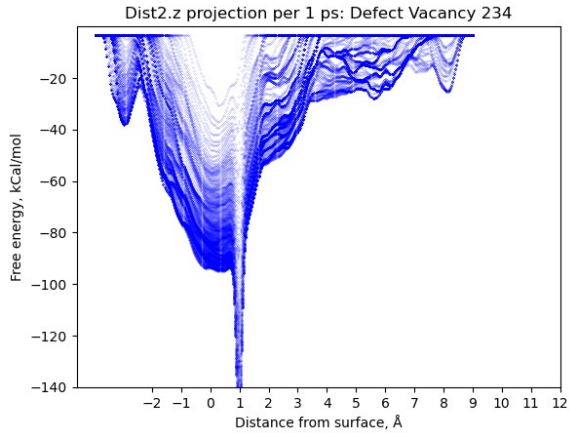
Vicinal 238



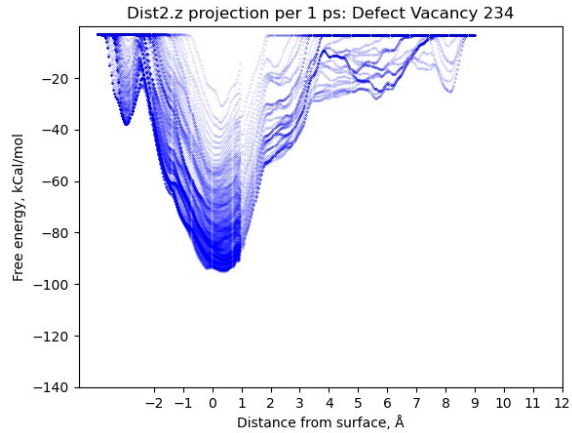


Defect Cases

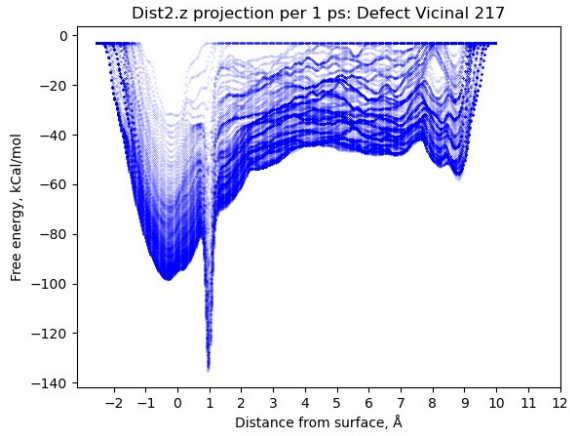
Original	Range-based projection
Geminal 234	Geminal 234
	
Vacancy 234	Vacancy 234



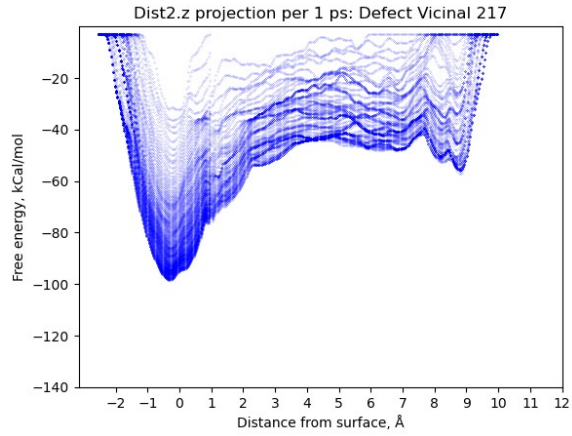
Vicinal 217



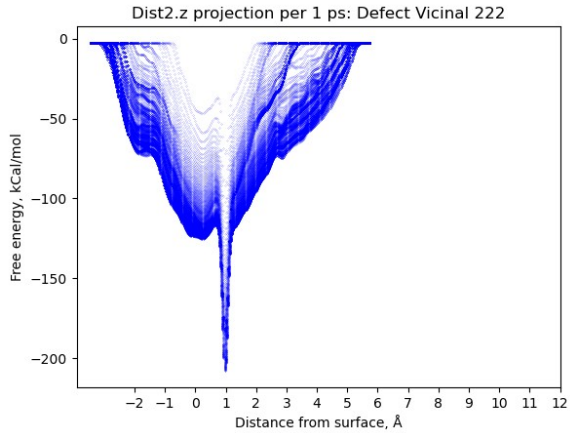
Vicinal 217



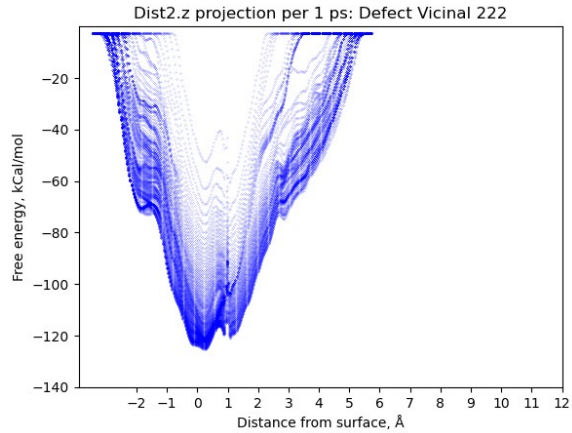
Vicinal 222



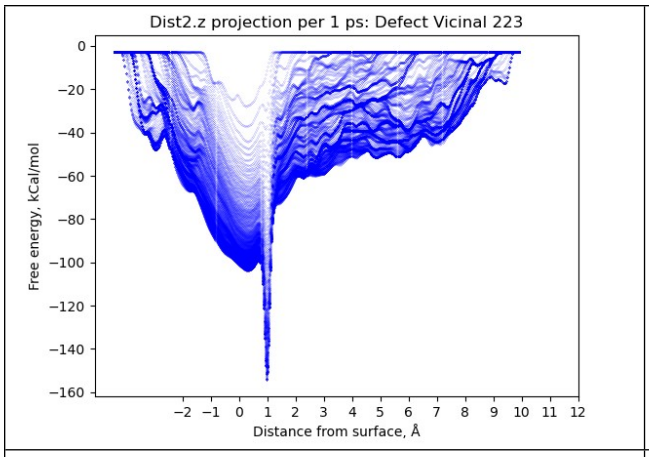
Vicinal 222

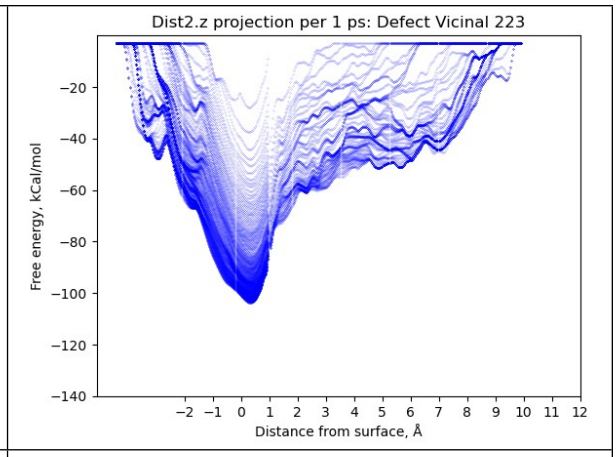


Vicinal 223



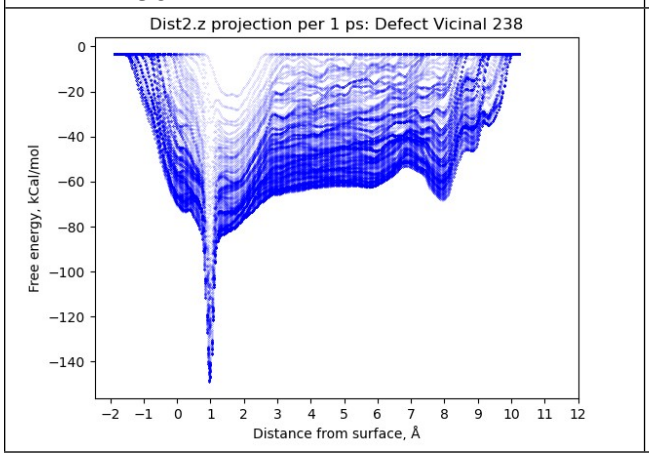
Vicinal 223





Vicinal 238

Vicinal 238



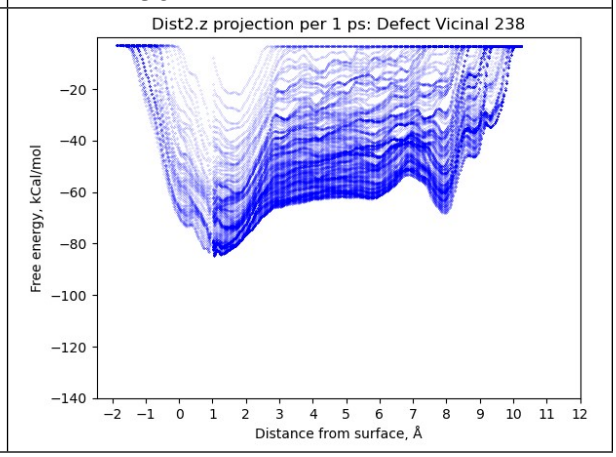
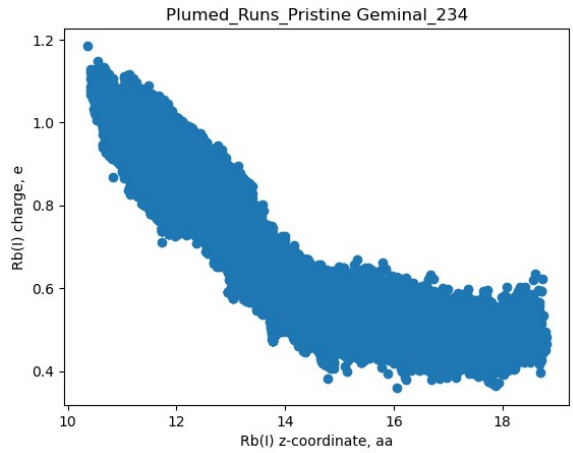
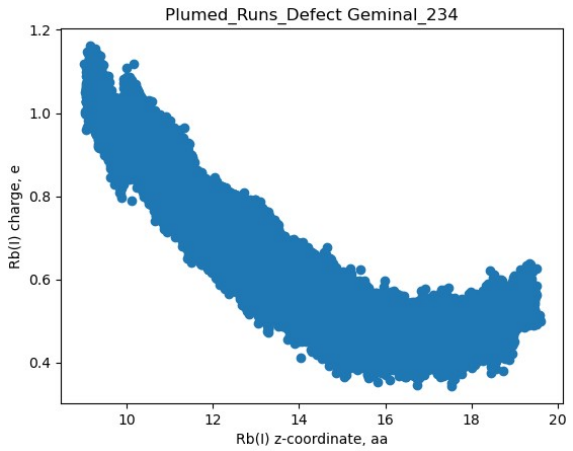
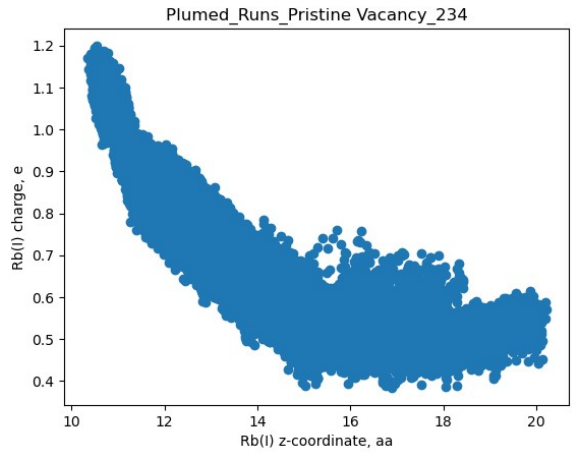
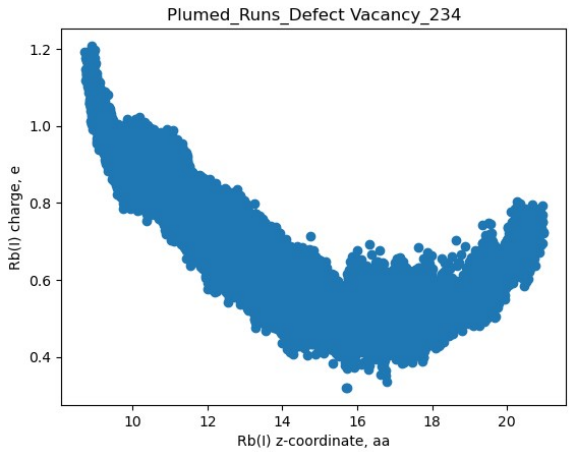
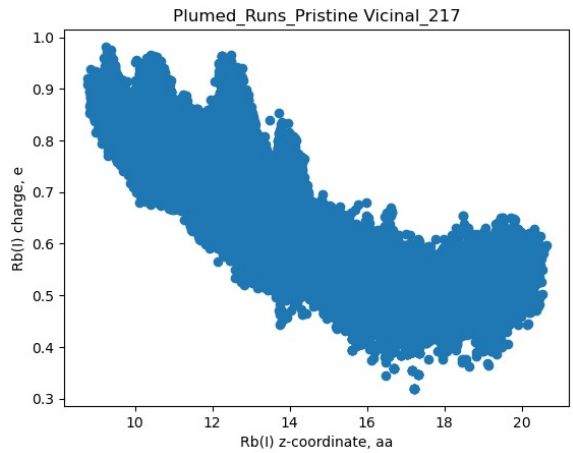
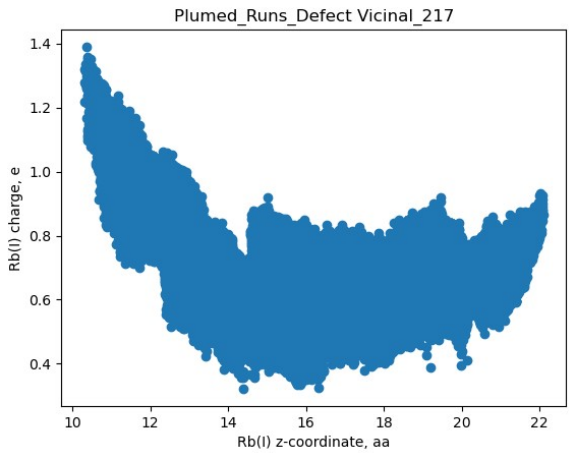


Table S8: Rb^+ Mulliken charge

As a function of distance, for trajectories of minimally 9.48 ns of sampling (pristine geminal 234). Rb^+ consistently charges as a function of distance to surface.

Pristine	Defect
Geminal 234	Geminal 234
	
Vacancy 234	Vacancy 234
	
Vicinal 217	Vicinal 217
	

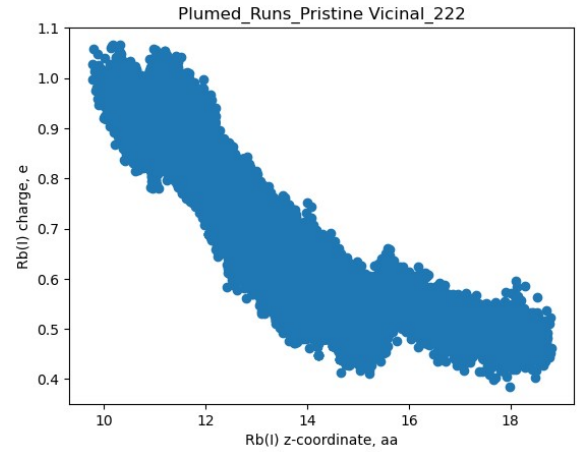
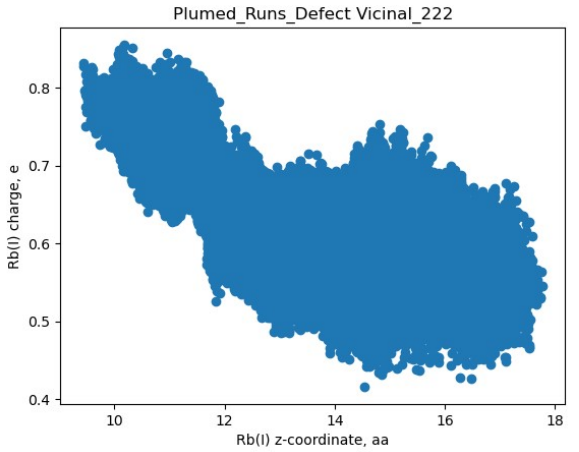
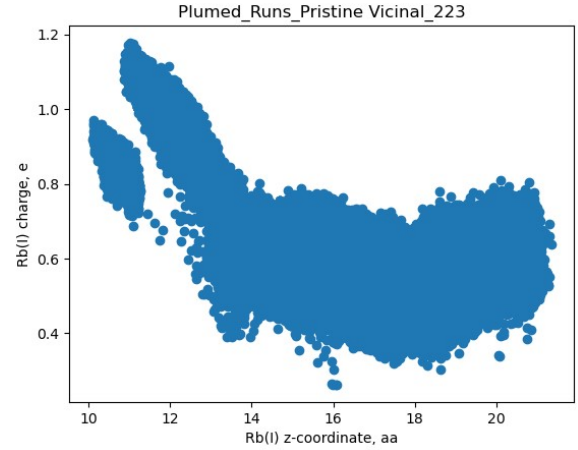
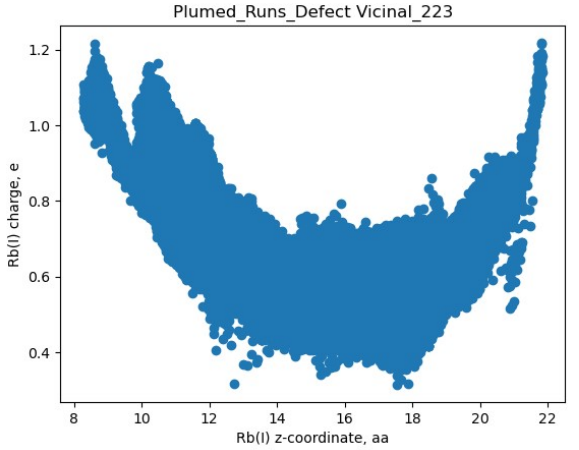
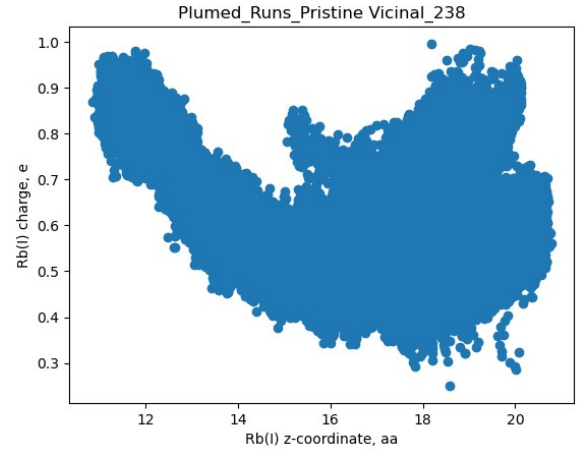
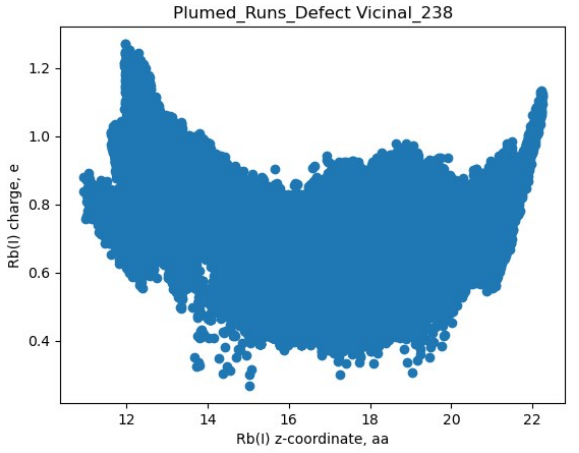
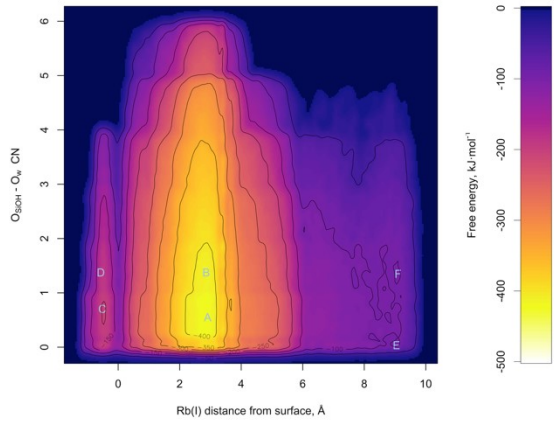
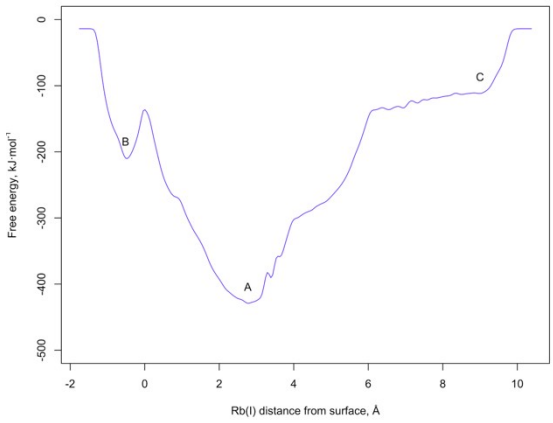
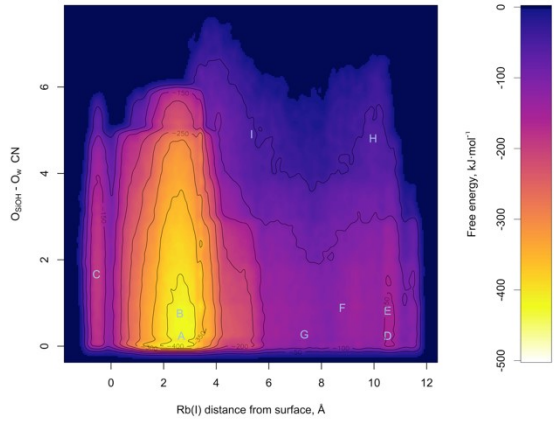
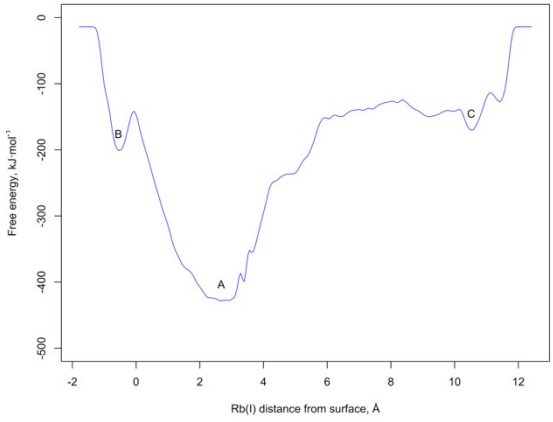
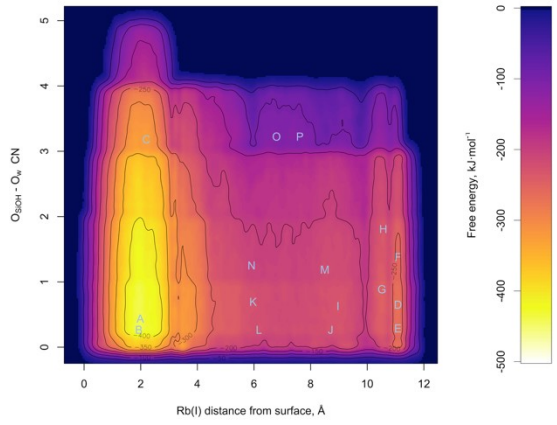
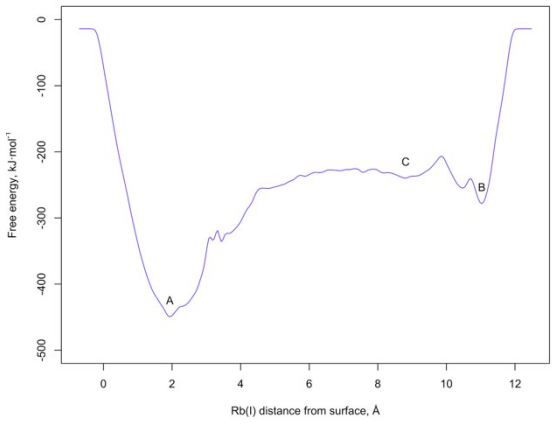
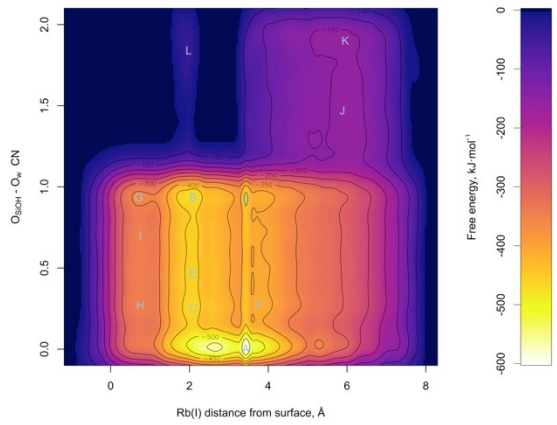
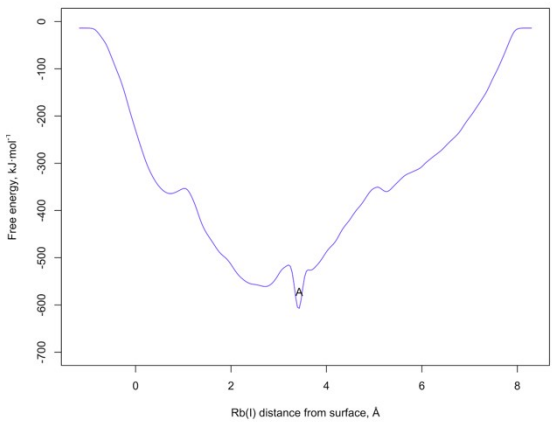
Vicinal 222	Vicinal 222
	
Vicinal 223	Vicinal 223
	
Vicinal 238	Vicinal 238
	

Table S9: Metadynminer FES

Defect systems

FES	Rb^+ distance projection
Geminal 234	Geminal 234
	
Vacancy 234	Vacancy 234
	
Vicinal 217	Vicinal 217
	

Vicinal 222	Vicinal 222
	
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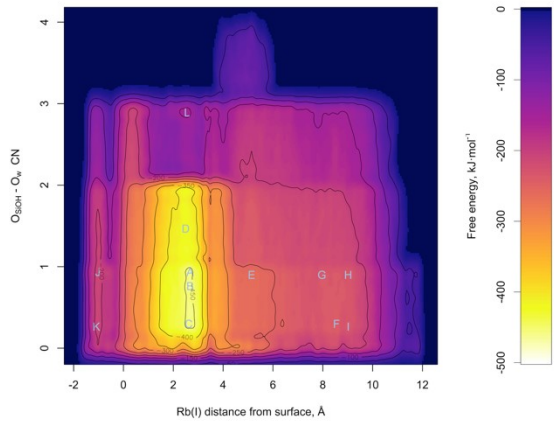
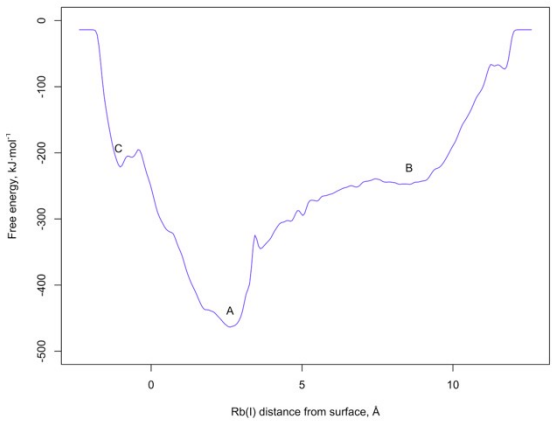
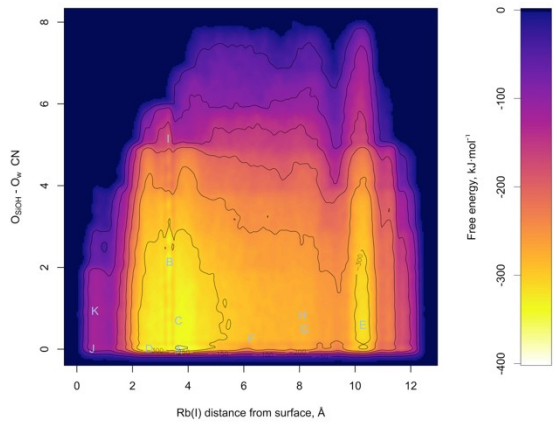
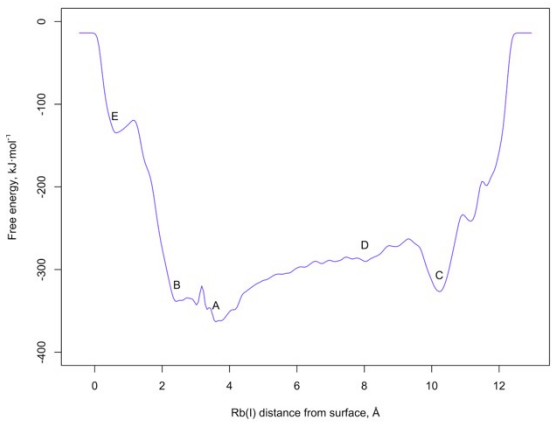
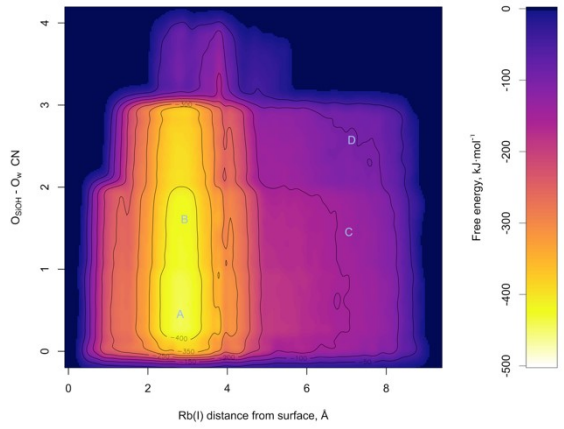
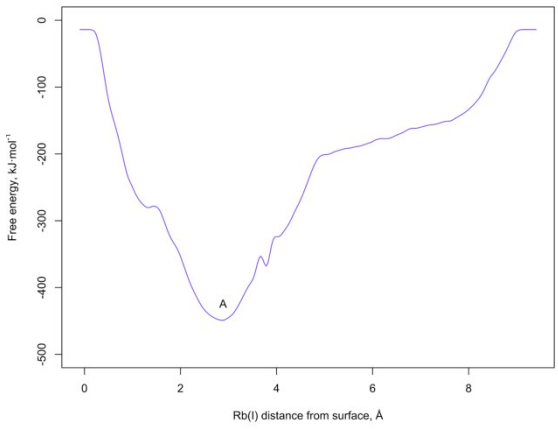
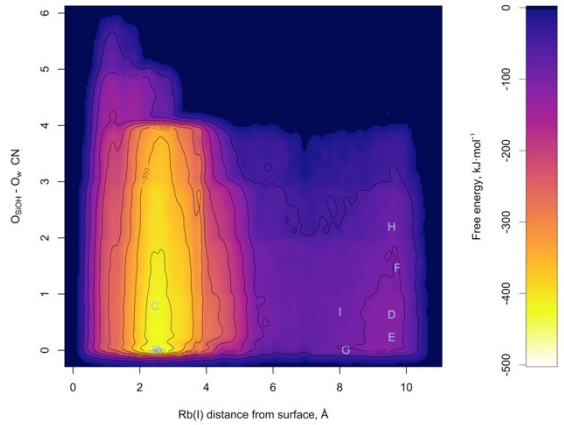
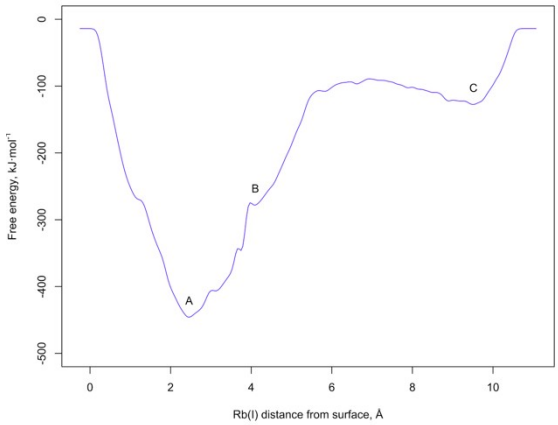
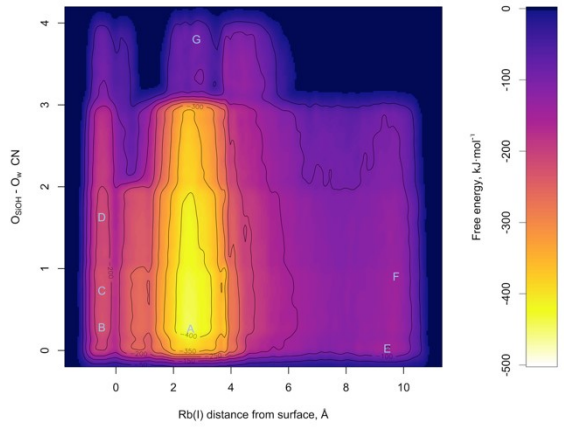
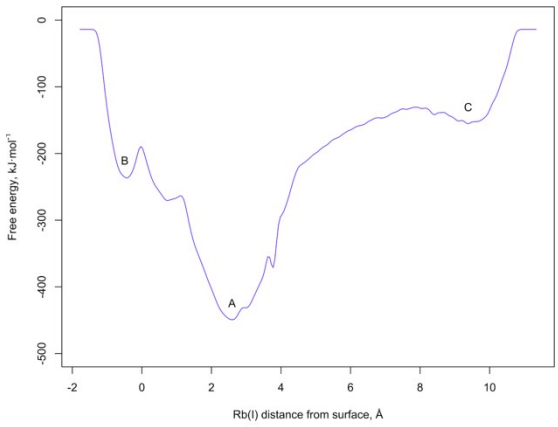
	
Vicinal 238	Vicinal 238
	

Pristine systems

FES	Rb^+ distance projection
Geminal 234	Geminal 234
	
Vacancy 234	Vacancy 234
	
Vicinal 217	Vicinal 217
	

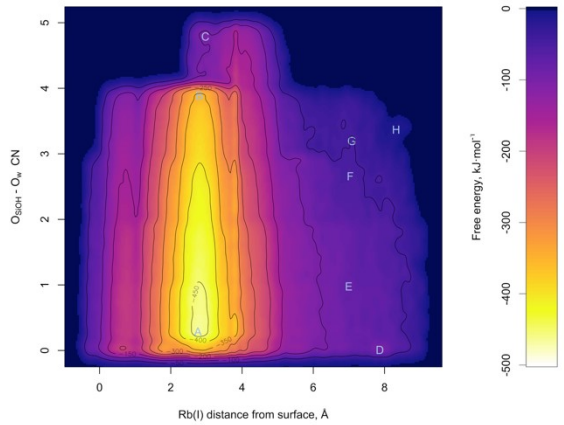
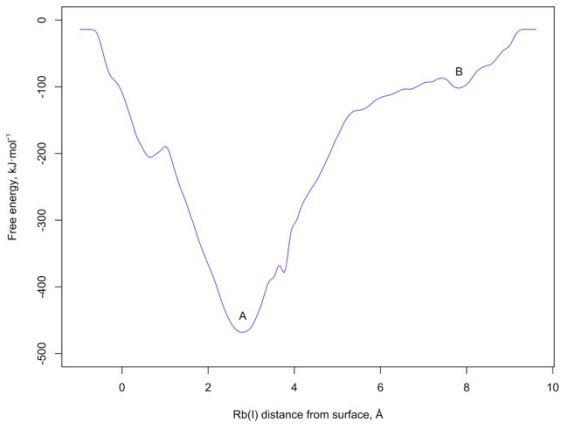
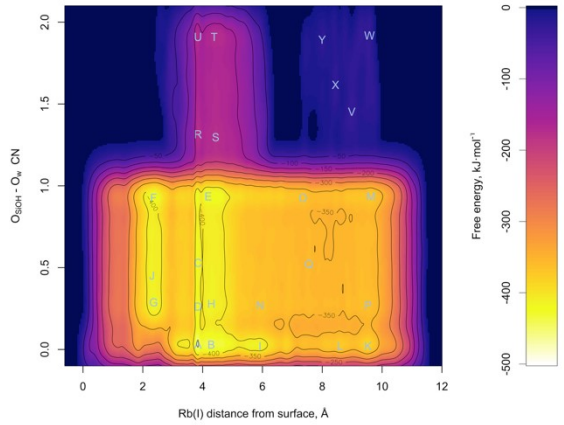
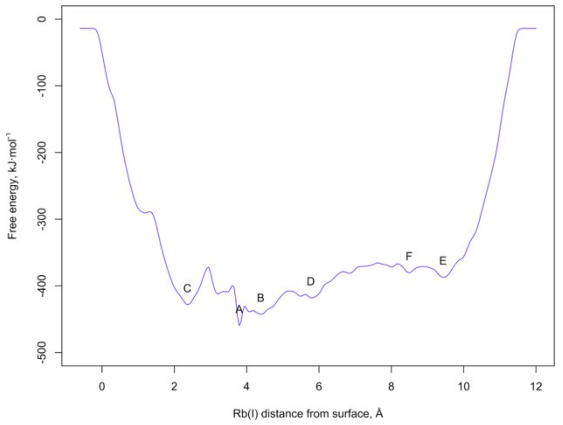
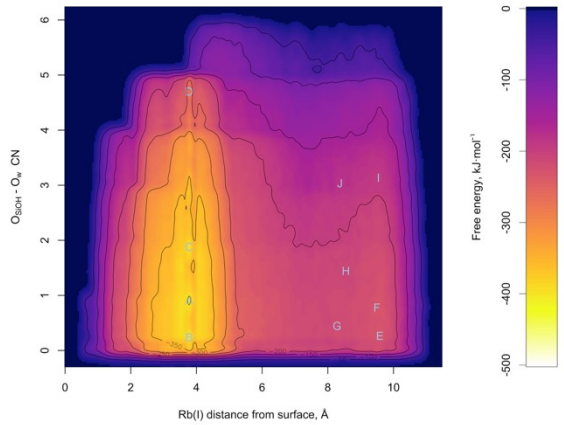
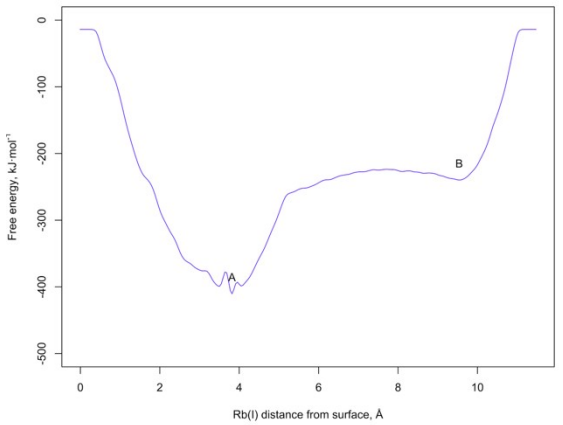
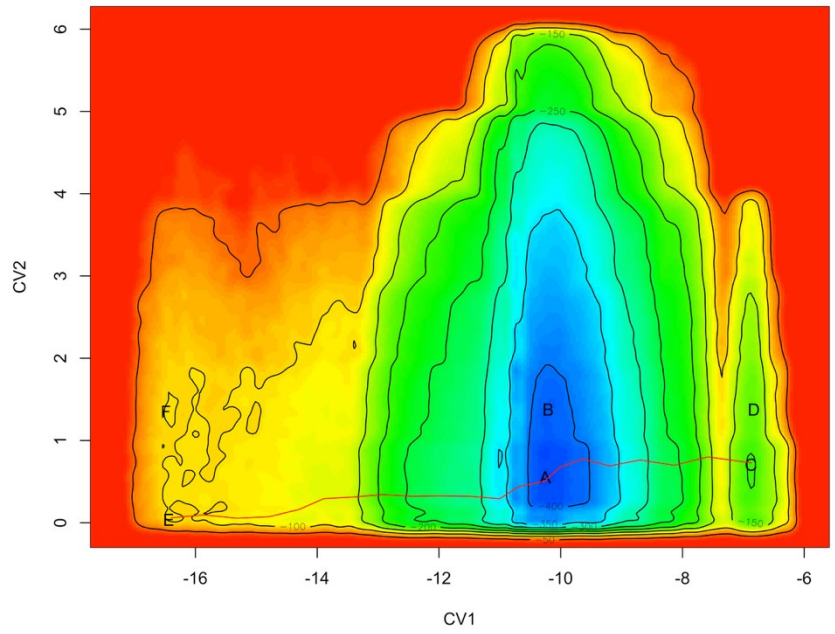
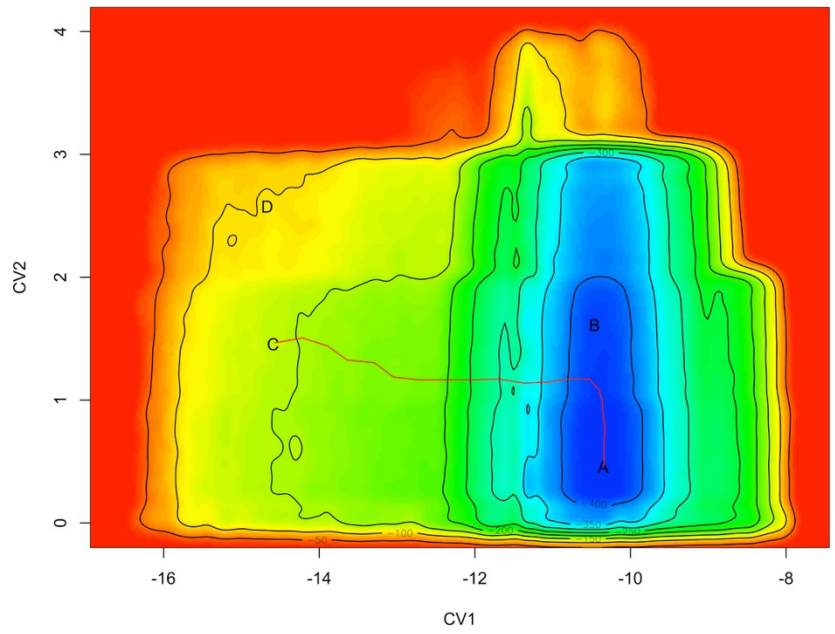
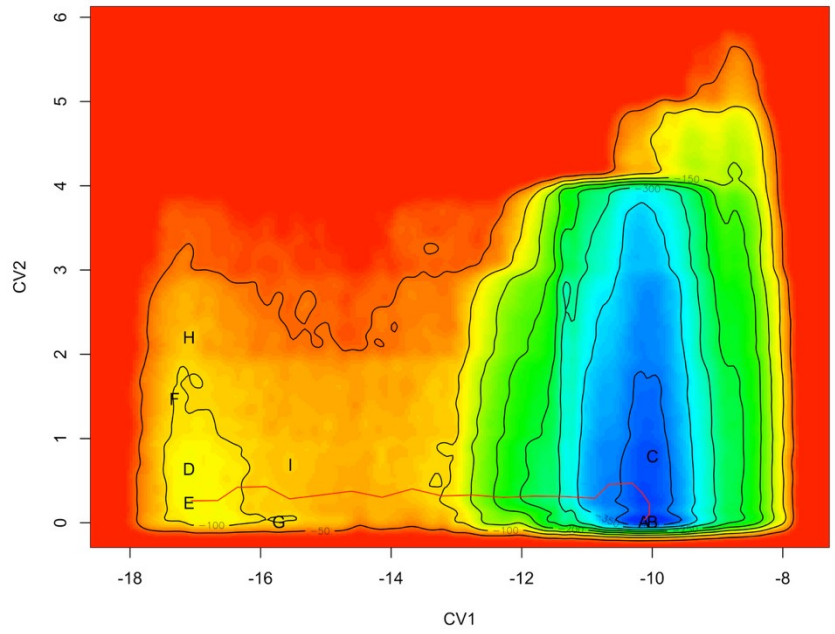
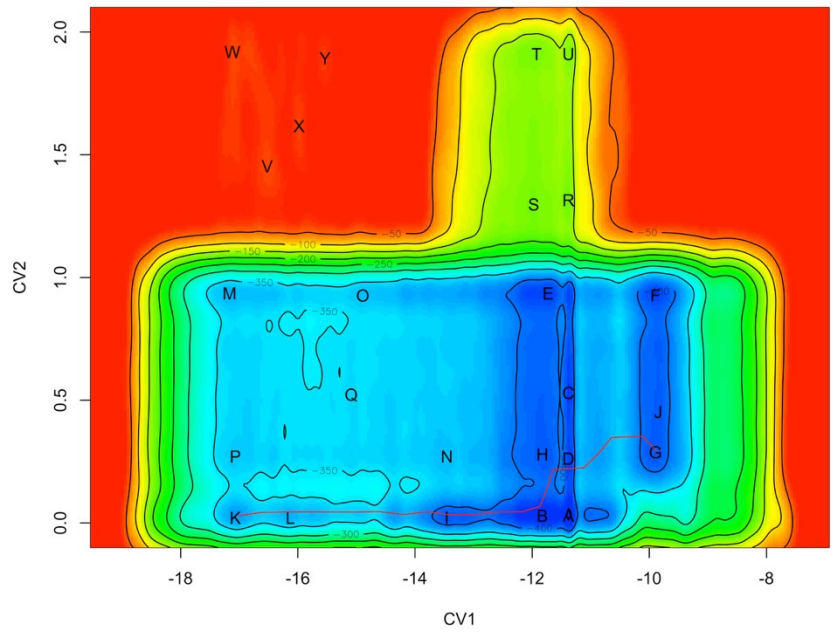
Vicinal 222	Vicinal 222
	
Vicinal 223	Vicinal 223
	
Vicinal 238	Vicinal 238
	

Table S10: Metadynminer Nudged Elastic Band

Defect Geminal 234

Pristine Geminal 234

Pristine Vacancy 234



Pristine Vicinal 223



Pristine Vicinal 238

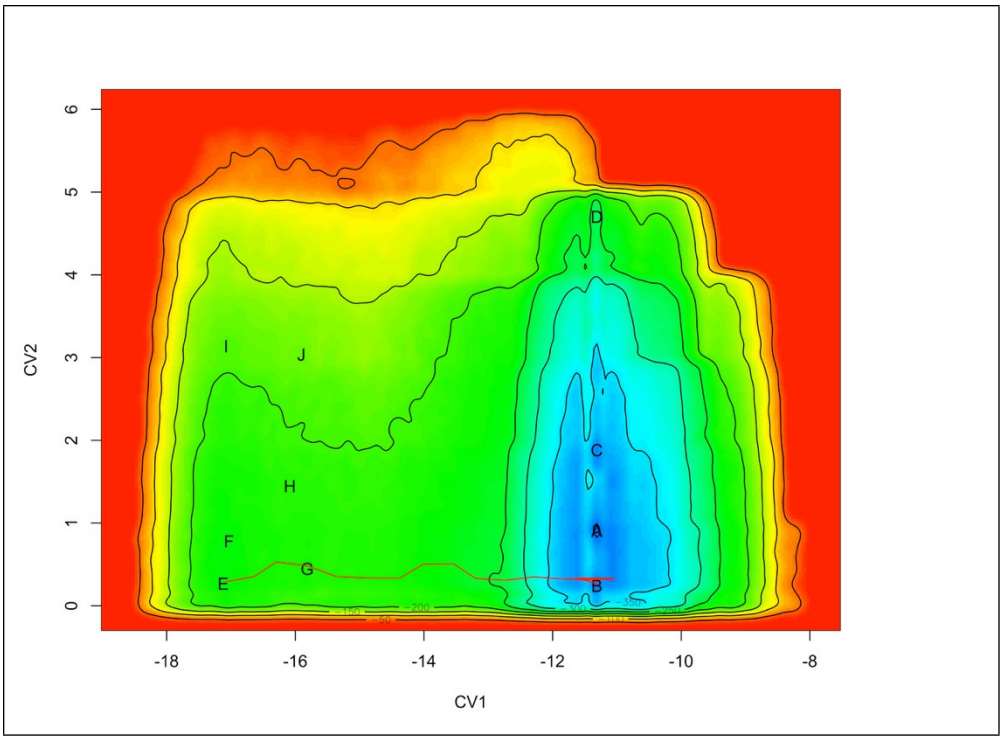

CV2
CV1
0
1
2
3
4
5
6
-18
-16
-14
-12
-10
-8
A
B
C
D
E
F
G
H
I
J

Table S11: Spearman for mechanistic insights

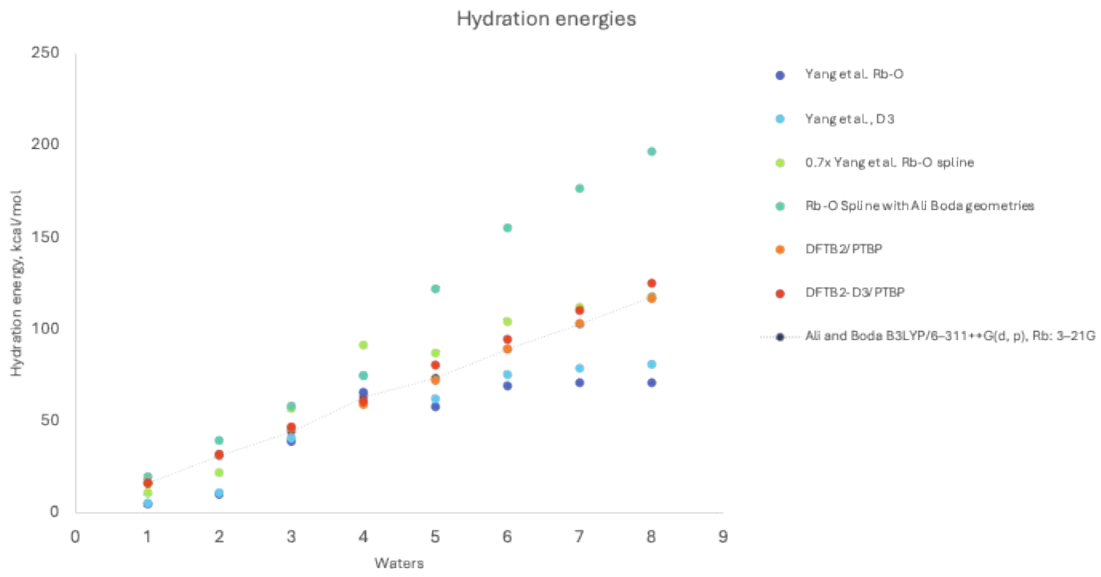
Note that the indices are indexed from zero rather than one, for example, Rb^+ 270 is index 269.

Defect			Spearman	Pristine			Spearman
Geminal_234	O-H-Rb bond	183, 18, 269	rho=0.5398 p=2.8018e-60	Geminal_234	O-H-Rb bond	79, 172, 275	rho = 0.3830, p = 1.1162e-27
						69, 166, 275	rho = 0.1258, p = 5.4215e-04
	Si-O-H-Rb torsion	263, 183, 18, 236	ρ=0.2460 p=3.1265e-12		Si-O-H-Rb torsion	163, 79, 172, 275	rho = 0.0005, p = 9.8942e-01
						157, 69, 166, 275	rho = 0.3490, p = 5.8443e-23
	Si-O-Si-O (below to silanol) torsion	263, 183, 1, 236	rho = -0.3837, p = 8.6219e-29		Si-O-Si-O (below to silanol) torsion	146, 66, 163, 79	rho = 0.1933, p = 9.1880e-08
						153, 61, 157, 69	rho = -0.0256, p = 4.8290e-01
Vacancy_234	O-H-Rb bond	183, 18, 269	rho = 0.4448, p = 2.0651e-39	Vacancy_234	O-H-Rb bond	79, 172, 275	rho = 0.2318, p = 8.8289e-11
						69, 166, 275	rho = 0.4703, p = 2.6205e-43
	Si-O-H-Rb torsion	263, 183, 18, 236	rho = 0.1876, p = 1.1833e-07		Si-O-H-Rb torsion	163, 79, 172, 275	0.1603, p = 8.4961e-06
						157, 69, 166, 275	rho = 0.1028, p = 4.4564e-03
	Si-O-Si-O (below to silanol) torsion	263, 183, 1, 236	rho = -0.5303, p = 3.8035e-58		Si-O-Si-O (below to silanol) torsion	146, 66, 163, 79	rho = 0.1294, p = 3.3482e-04
						153, 61, 157, 69	rho = 0.4267, p = 3.6867e-35
Vicinal_217	O-H-Rb bond	179, 1, 269	rho = -0.1518, p = 1.9226e-05	Vicinal_217	O-H-Rb bond	77, 170, 275	rho = -0.1364, p = 1.5339e-04
	Si-O-H-Rb torsion	263, 179, 1, 269	rho = 0.0152, p = 6.7129e-01		Si-O-H-Rb torsion	161, 77, 170, 275	rho = -0.0884, p = 1.4411e-02

	Si-O-Si-O (below to silanol) torsion	259, 172, 263, 179	rho = 0.1314, p = 2.1999e-04		Si-O-Si-O (below to silanol) torsion	155, 63, 161, 77	rho = -0.5459, p = 1.0268e-60
Vicinal_222	O-H-Rb bond	187, 5, 269	rho = 0.1828, p = 2.2410e-07	Vicinal_222	O-H-Rb bond	71, 168, 275	rho = 0.5443, p = 1.1208e-58
	Si-O-H-Rb torsion	267, 187, 5, 269	rho = -0.0250, p = 4.8334e-01		Si-O-H-Rb torsion	159, 71, 168, 275	rho = -0.4426, p = 4.3888e-37
	Si-O-Si-O (below to silanol) torsion	251, 155, 267, 187	rho = 0.1543, p = 1.3076e-05		Si-O-Si-O (below to silanol) torsion	155, 63, 159, 71	rho = 0.7447, p = 1.2369e-132
Vicinal_223	O-H-Rb bond	No preferred adsorption.		Vicinal_223	O-H-Rb bond	69, 166, 275	rho = 0.6648, p = 1.3885e-96
	Si-O-H-Rb torsion				Si-O-H-Rb torsion	157, 69, 166, 275	rho = -0.1047, p = 4.1475e-03
	Si-O-Si-O (below to silanol) torsion				Si-O-Si-O (below to silanol) torsion	153, 61, 157, 69	rho = -0.4326, p = 1.8560e-35
Vicinal_238	O-H-Rb bond	179, 1, 269	rho = 0.5070, p = 4.3298e-53	Vicinal_238	O-H-Rb bond	77, 170, 275	rho = 0.5378, p = 3.2536e-57
	Si-O-H-Rb torsion	263, 179, 1, 269	rho = -0.1957, p = 2.7238e-08		Si-O-H-Rb torsion	161, 77, 170, 275	rho = -0.4217, p = 1.4596e-33
	Si-O-Si-O (below to silanol) torsion	259, 171, 263, 179	rho = 0.1600, p = 5.8618e-06		Si-O-Si-O (below to silanol) torsion	155, 63, 161, 77	rho = -0.4461, p = 8.3317e-38

Figure S2: Hydration energies

$Rb^+ + XH_2O \rightarrow Rb(H_2O)X^+$



Comparison across modifications to the Yang *et al.*[6] parameters and the periodic table baseline parameter set (PTBP).[7] We find that the Yang *et al.*[6] underpredicts the hydration energies of Rb^+ hydrates of five waters or more.

Table S12: Mean absolute errors in kcal·mol-1 for hydration energies

MAE against hydration energies from Boda and Ali.[8]

Yang et al. params	Yang et al. params, D3	0.7x Yang et al. Rb-O spline	Rb-O Spline with Boda and Ali geometries	DFTB2/PTBP	DFTB2-D3/PTBP
19.3382556	16.5737563	11.6131887	37.967573	1.02536368	4.1595272

For hydration energies, the DFTB2/PTBP performs most similarly to the Boda and Ali B3LYP/6–311++G(d, p), Rb: 3–21G, with the parameters in this work showing large errors for hydration errors, with Grimme D3 dispersion[9] improving the errors by 3 $kcal \cdot mol^{-1}$ but not improving the trend of underpredicting the hydration energies of high hydrates, (pentaquo and above).

Figure S3: Rb^+ coordination at surface for the Defect Geminal 234 system

Sampled from minimally 15 ps trajectories starting from the stationary points in the defect geminal 234 system in the main manuscript Figure 2, near the surface in Figure S3 and solvated away from the surface in Figure S4. All simulations were down-sampled randomly in the plotted range so that all simulations show the same number of points. Near the surface, the original parameters show a higher coordination to water oxygens than the other models, at 3- rather than 2-coordinate, but is otherwise consistent for the total Rb^+ coordination to silanol and quartz oxygen and total coordination to oxygen.

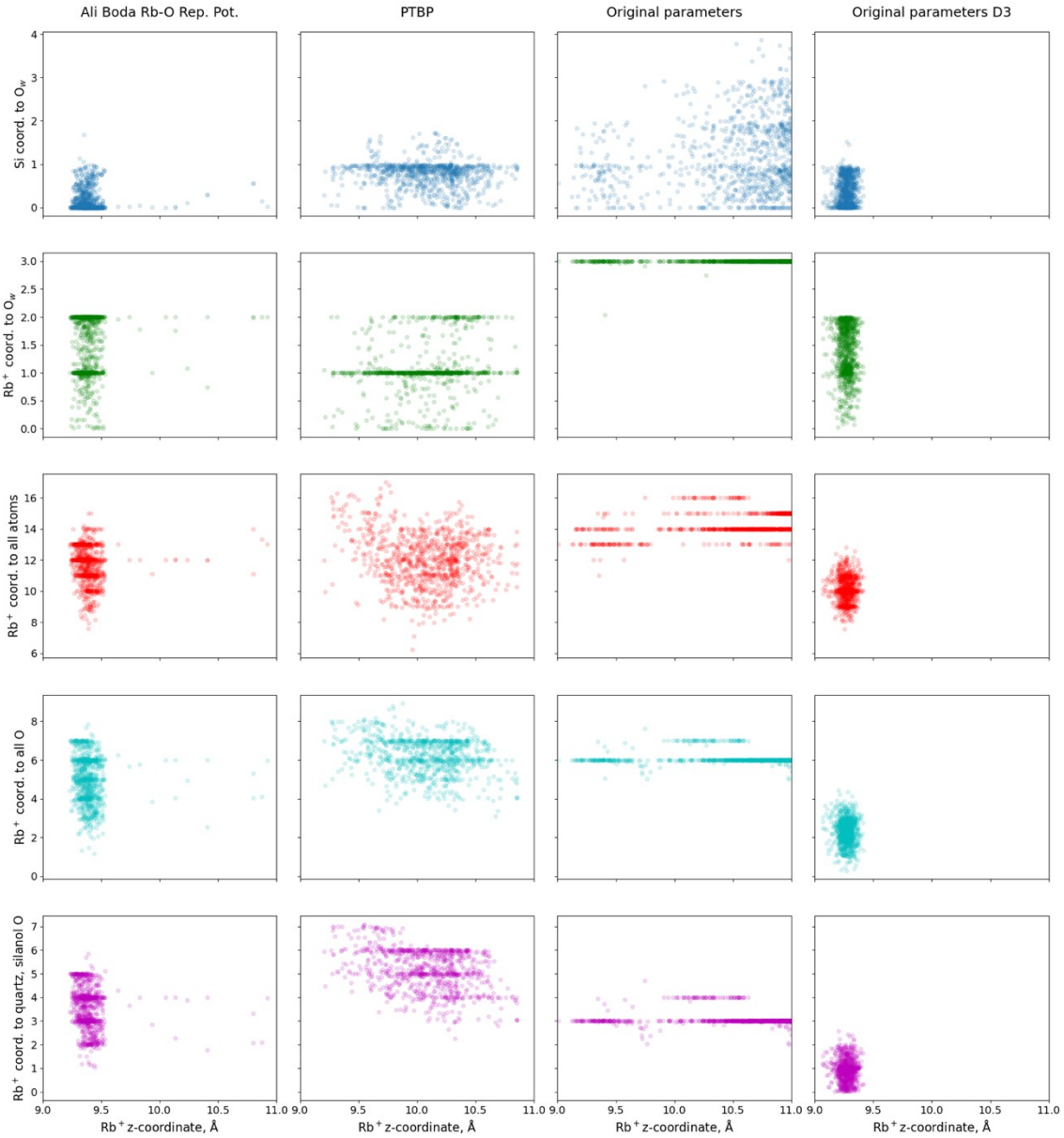


Figure S4: Solvated Rb^+ coordination for the Defect Geminal 234 system

Sampled from minimally 15 ps trajectories starting from the stationary points in the defect geminal 234 system in the main manuscript Figure 2, solvated away from the surface in Figure S4. All simulations were down-sampled randomly in the plotted range so that all simulations show the same number of points. Far from the surface, the original parameters show a lower coordination to water oxygens than the other models, at 3- rather than (4-8)-coordinate. The quartz and silanol coordination in the models is from interactions across the periodic reflection. D3 dispersion increases the Rb^+ coordination to all oxygen, improving the description of the solvated Rb^+. The Boda and Ali comparison is to a repulsive potential fitted to the geometries reported by Boda and Ali.[8] A comparison across spline repulsive potentials is given in Figure S6.

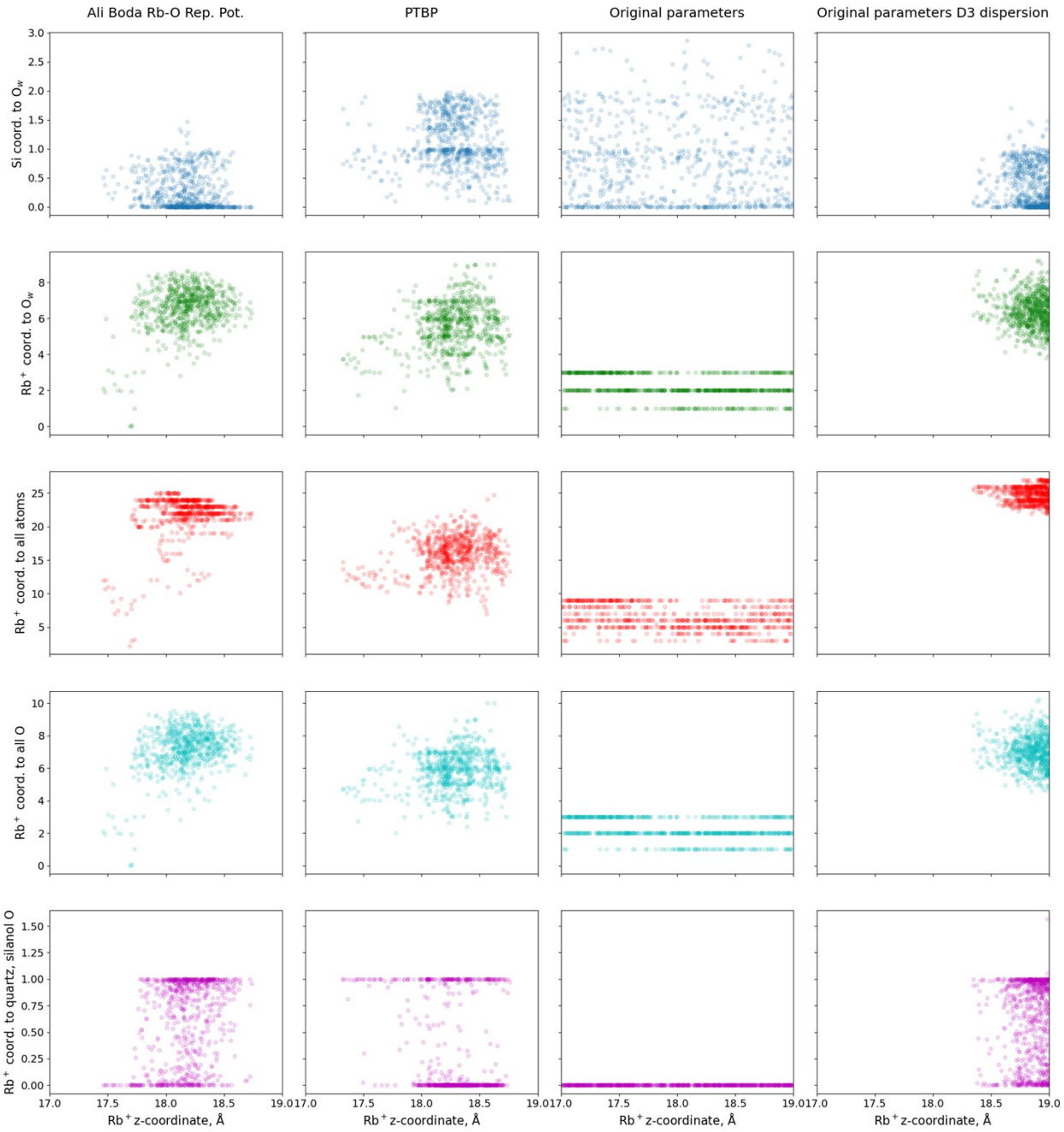
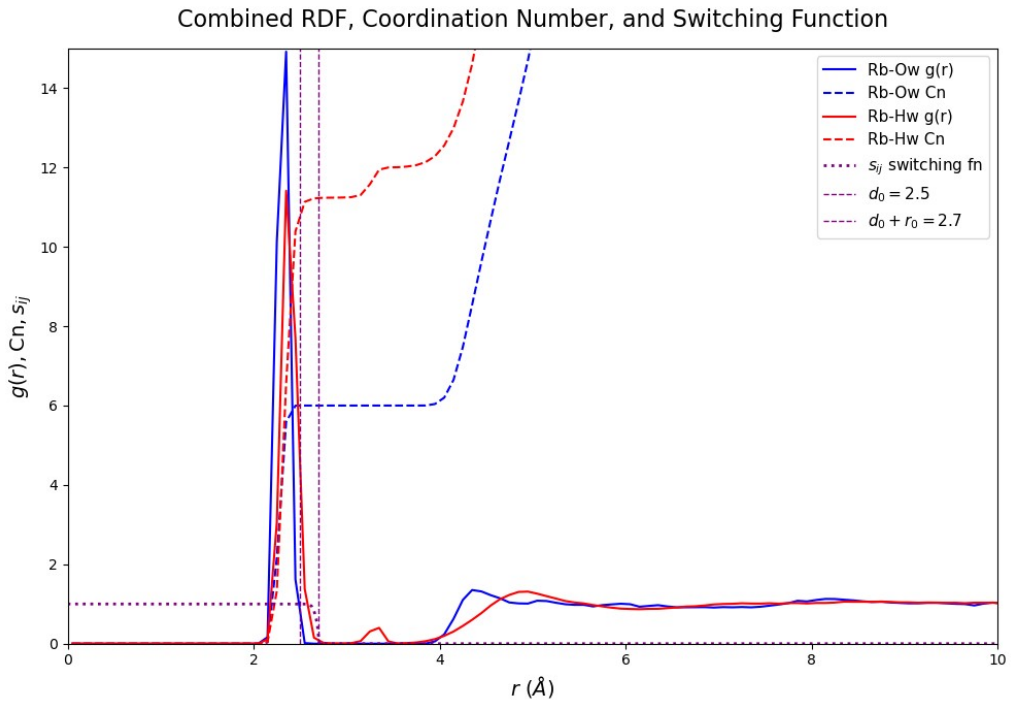

Ali Boda Rb-O Rep. Pot.
PTBP
Original parameters
Original parameters D3 dispersion
Si coord. to O_w
Rb^+ coord. to O_w
Rb^+ coord. to all atoms
Rb^+ coord. to all O
Rb^+ coord. to quartz, silanol O
Rb^+ z-coordinate, Å

Figure S5: RDF and coordination switching function for original parameters

A



B

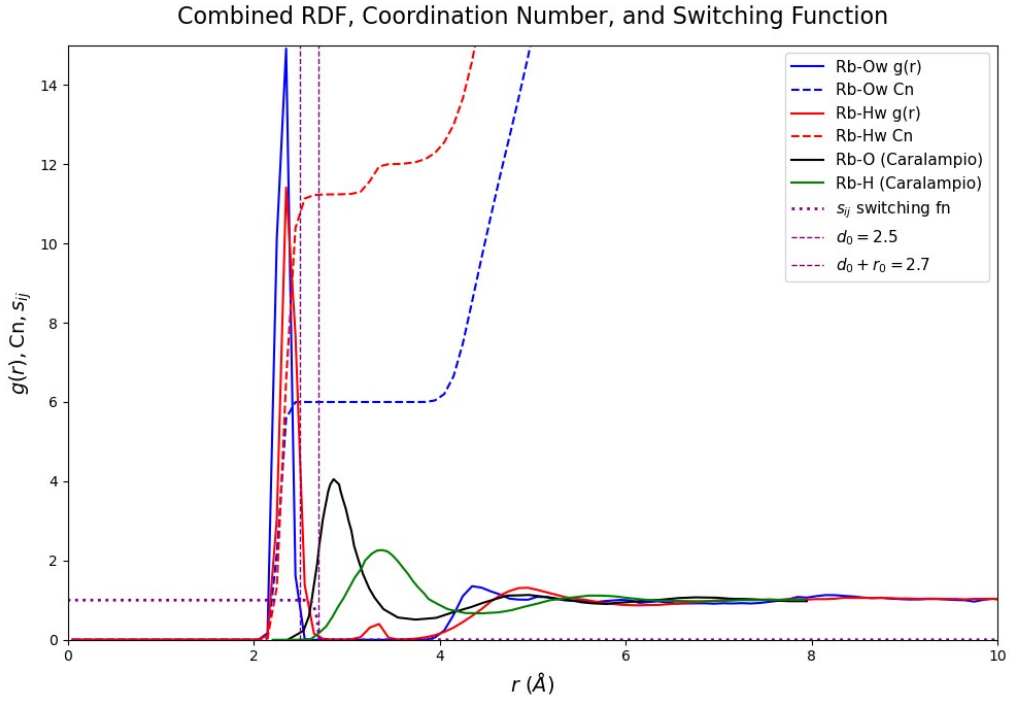
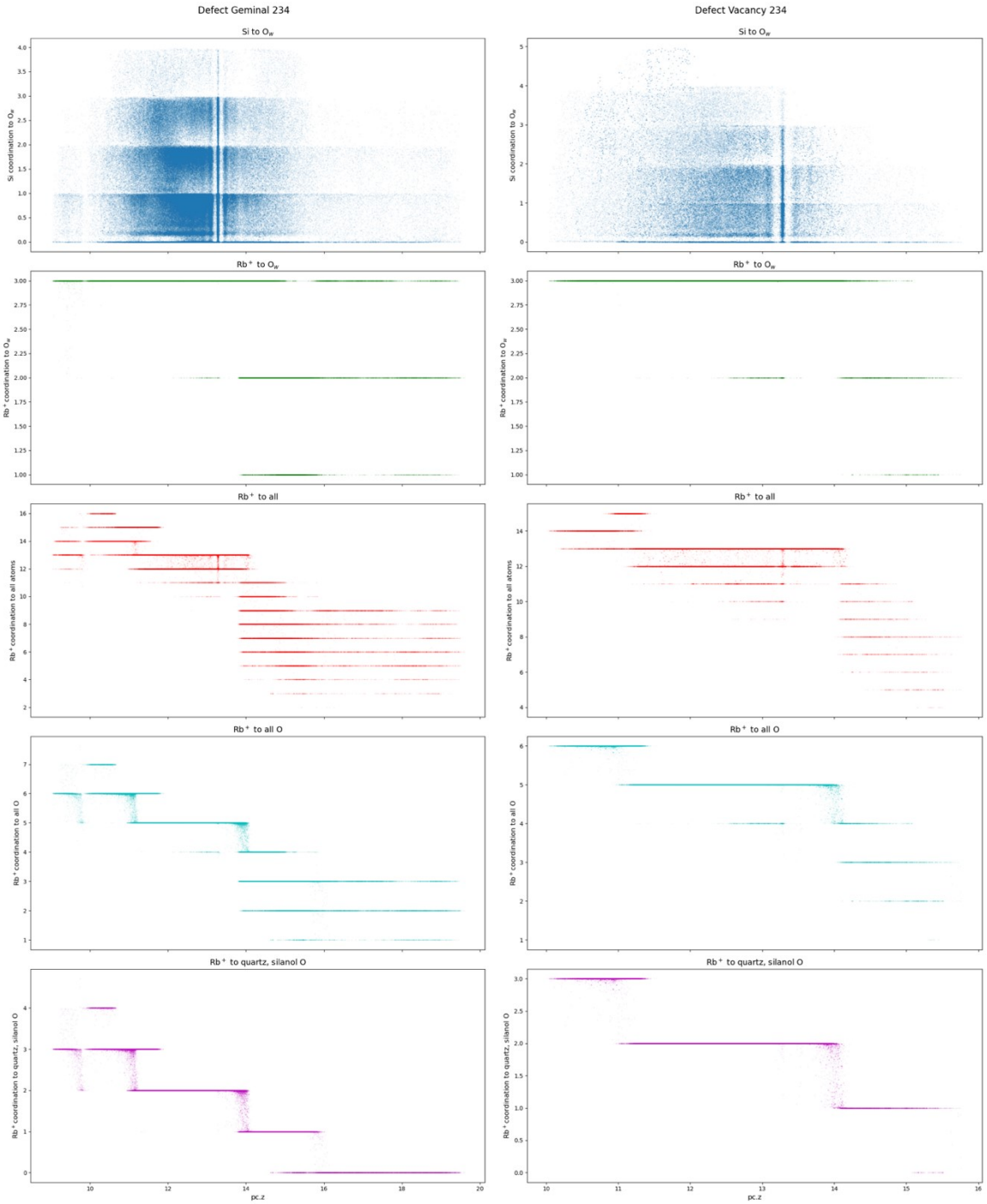
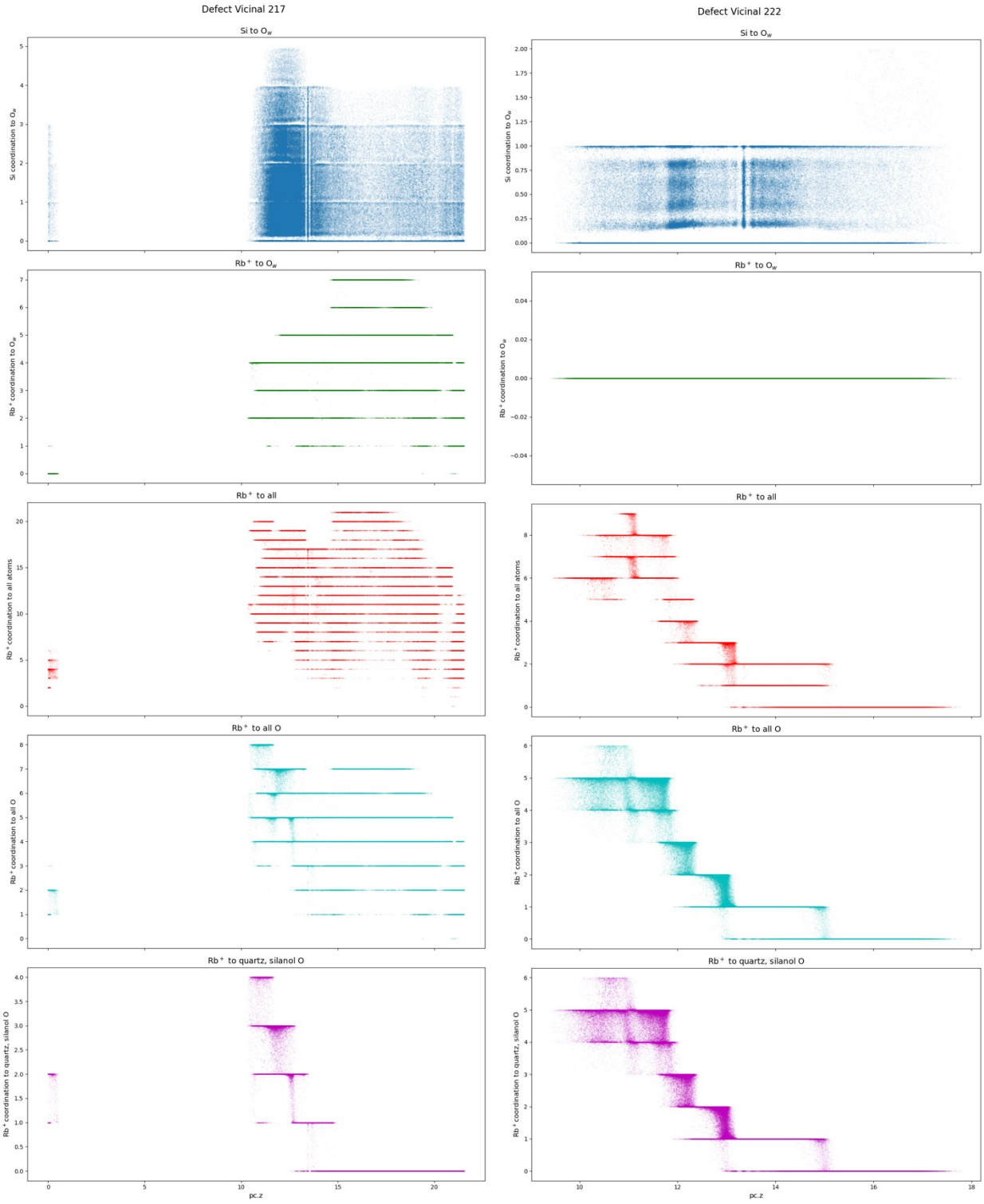


Figure S5 includes the radial distribution function (solid), coordination number (dashed), and PLUMED coordination switching function (dashed, purple) for a 60-ps simulation of RbOH in bulk water, without the quartz surface. These values were used as the cutoff for the original parameter set in Figures S3-S4 and Tables S13-S14. For the other parameter combinations, the optimized geometry bond length of the 8-coordinate complex was used as the radial cutoff for the coordination switching function, with 0.2 r_0 damped decay in all cases. We see that the Rb-O and Rb-H distance is substantially shorter than those reported by Caralampio *et al.,*[10] plotted in (B), with 2.34 vs. 2.85 Å for Rb-O and 2.36 vs. 3.37 Å for Rb-H.

Table S13: Rb^+ coordination to all atoms, water, quartz, and silanol oxygen for defect systems

Analogous plots to Figures S3 and S4 for the full trajectories with the original parameters. Frames were assessed with PLUMED driver, corresponding to every 20 fs.




Defect Vicinal 217
Defect Vicinal 222
Si to O_w
Rb^+ to O_w
Rb^+ to all
Rb^+ to all O
Rb^+ to quartz, silanol O
Si coordination to O_w
Rb^+ coordination to O_w
Rb^+ coordination to all atoms
Rb^+ coordination to all O
Rb^+ coordination to quartz, silanol O
pc.z

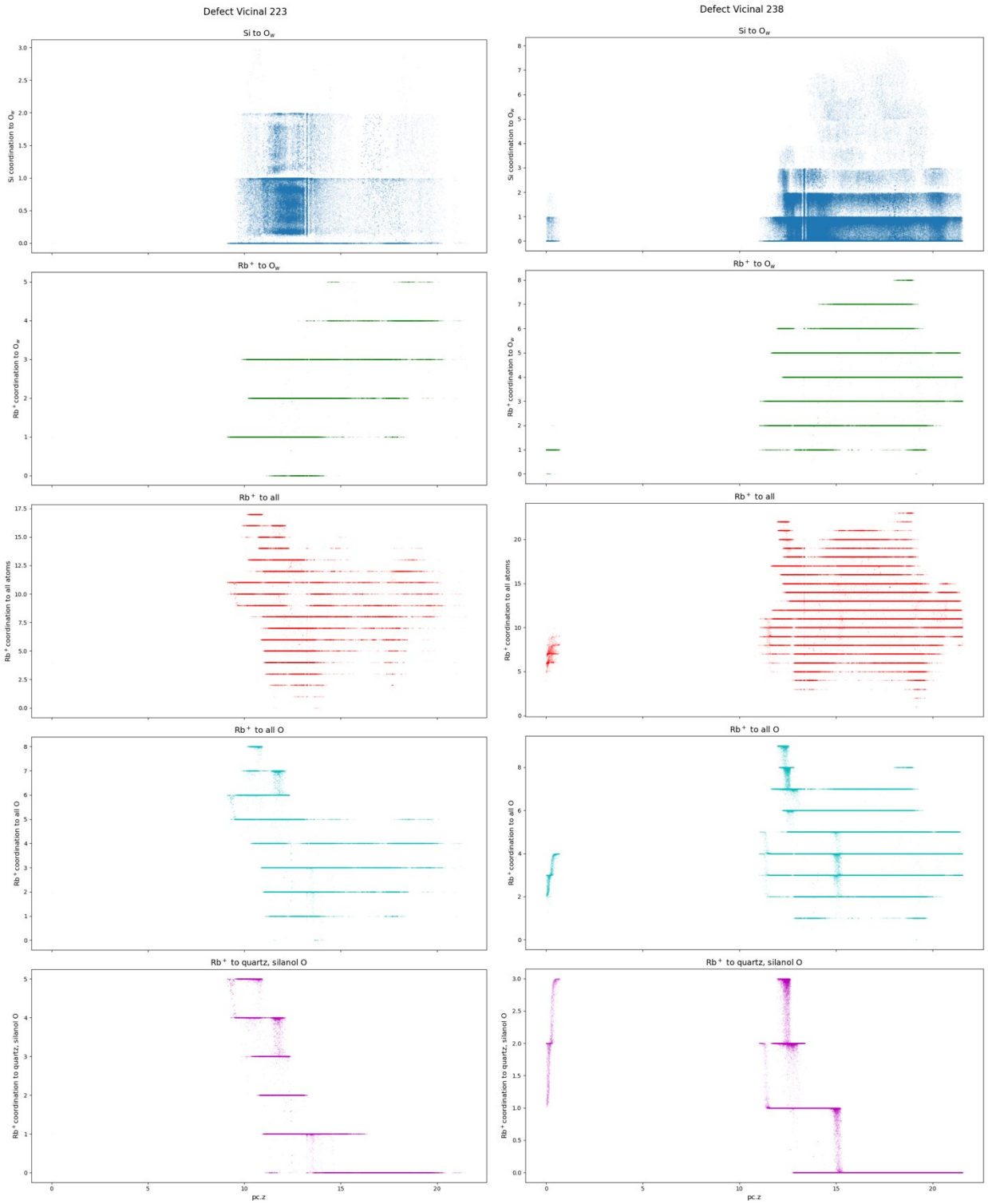
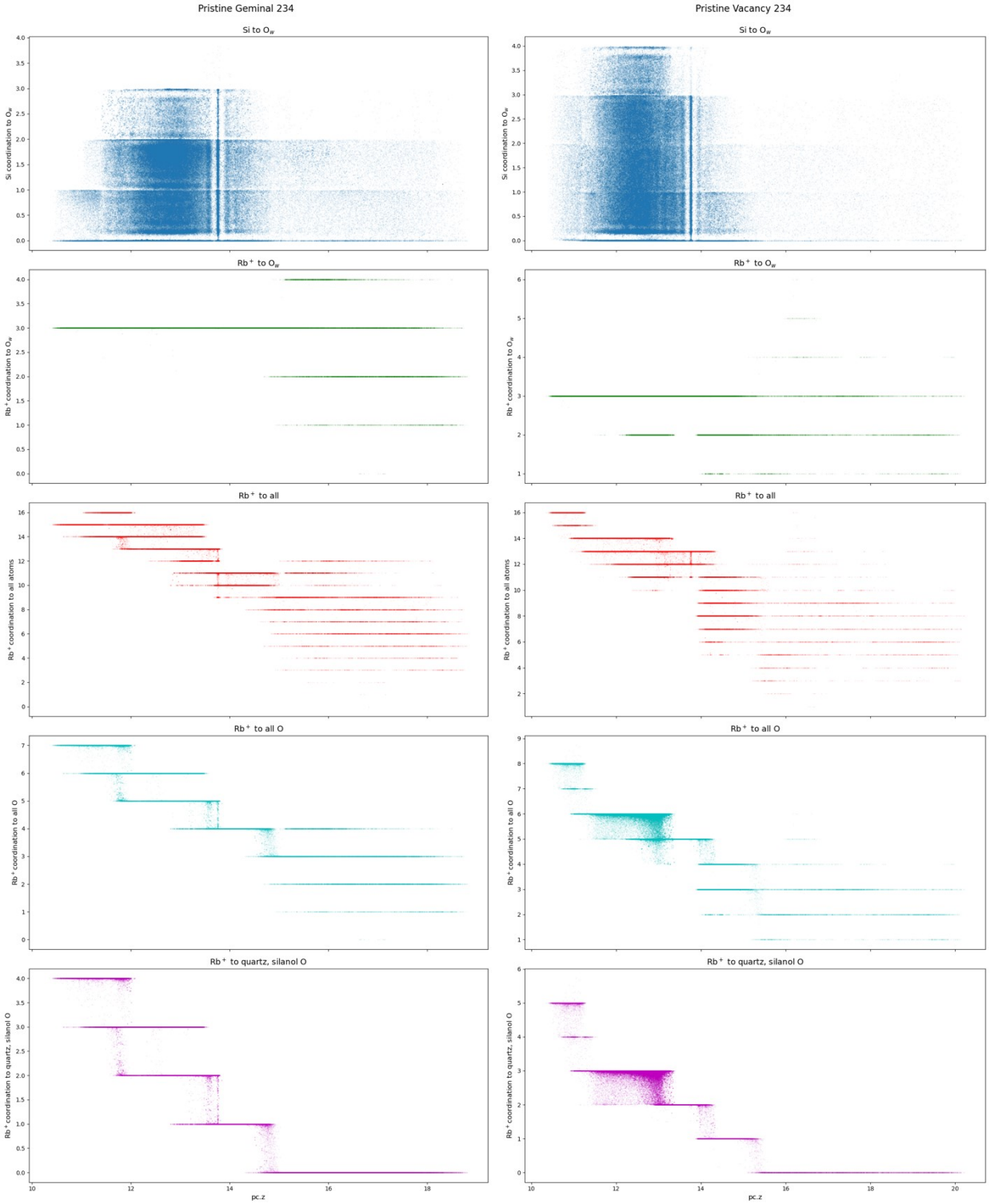
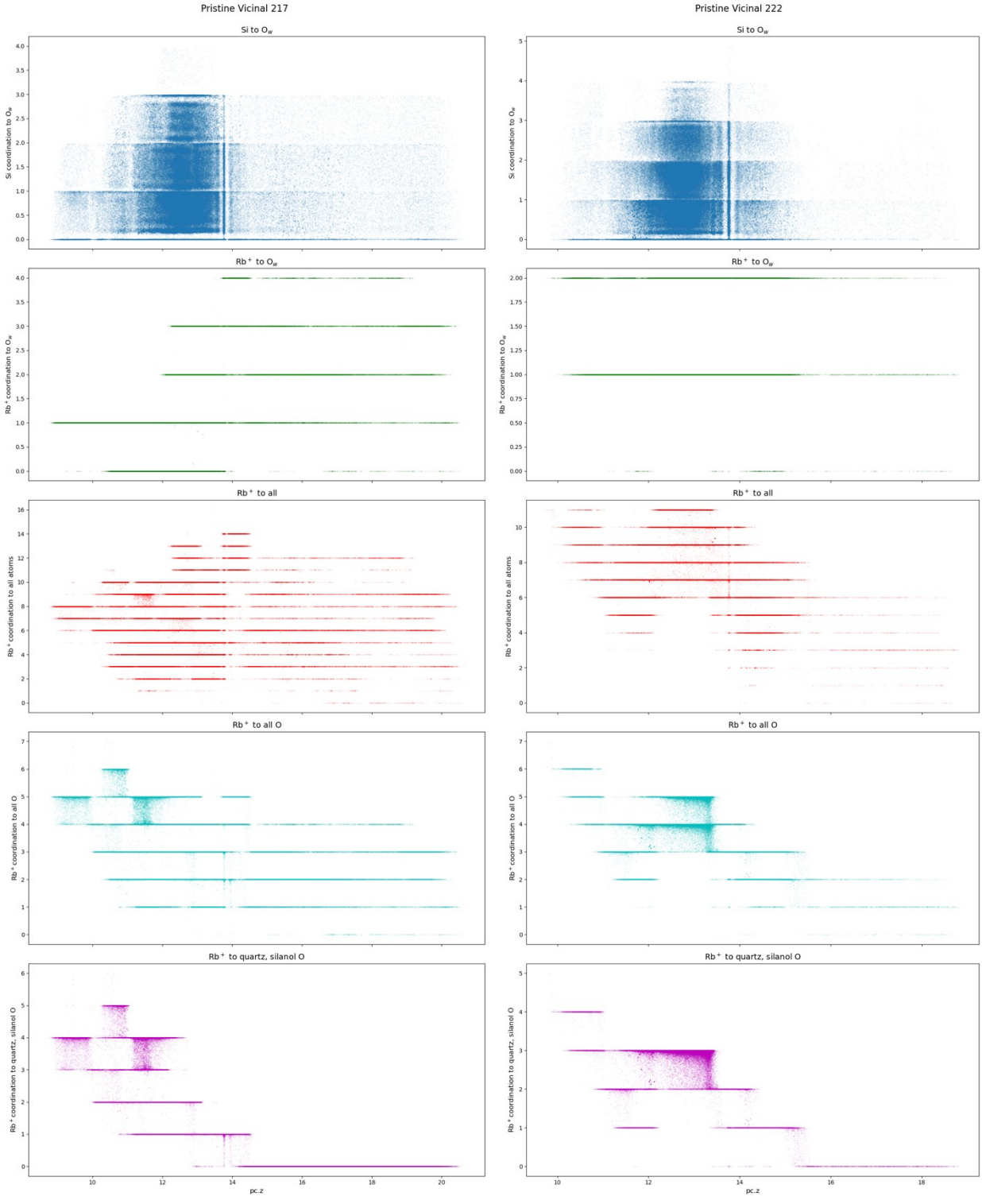

Defect Vicinal 223
Defect Vicinal 238
Si to O_w
Rb^+ to O_w
Rb^+ to all
Rb^+ to all O
Rb^+ to quartz, silanol O
Si coordination to O_w
Rb^+ coordination to O_w
Rb^+ coordination to all atoms
Rb^+ coordination to all O
Rb^+ coordination to quartz, silanol O
pc.z

Table S14: Rb^+ coordination to all atoms, water, quartz, and silanol oxygen for pristine systems




Pristine Vicinal 217
Pristine Vicinal 222
Si to O_w
Rb^+ to O_w
Rb^+ to all
Rb^+ to all O
Rb^+ to quartz, silanol O
Si coordination to O_w
Rb^+ coordination to O_w
Rb^+ coordination to all atoms
Rb^+ coordination to all O
Rb^+ coordination to quartz, silanol O
pc.z

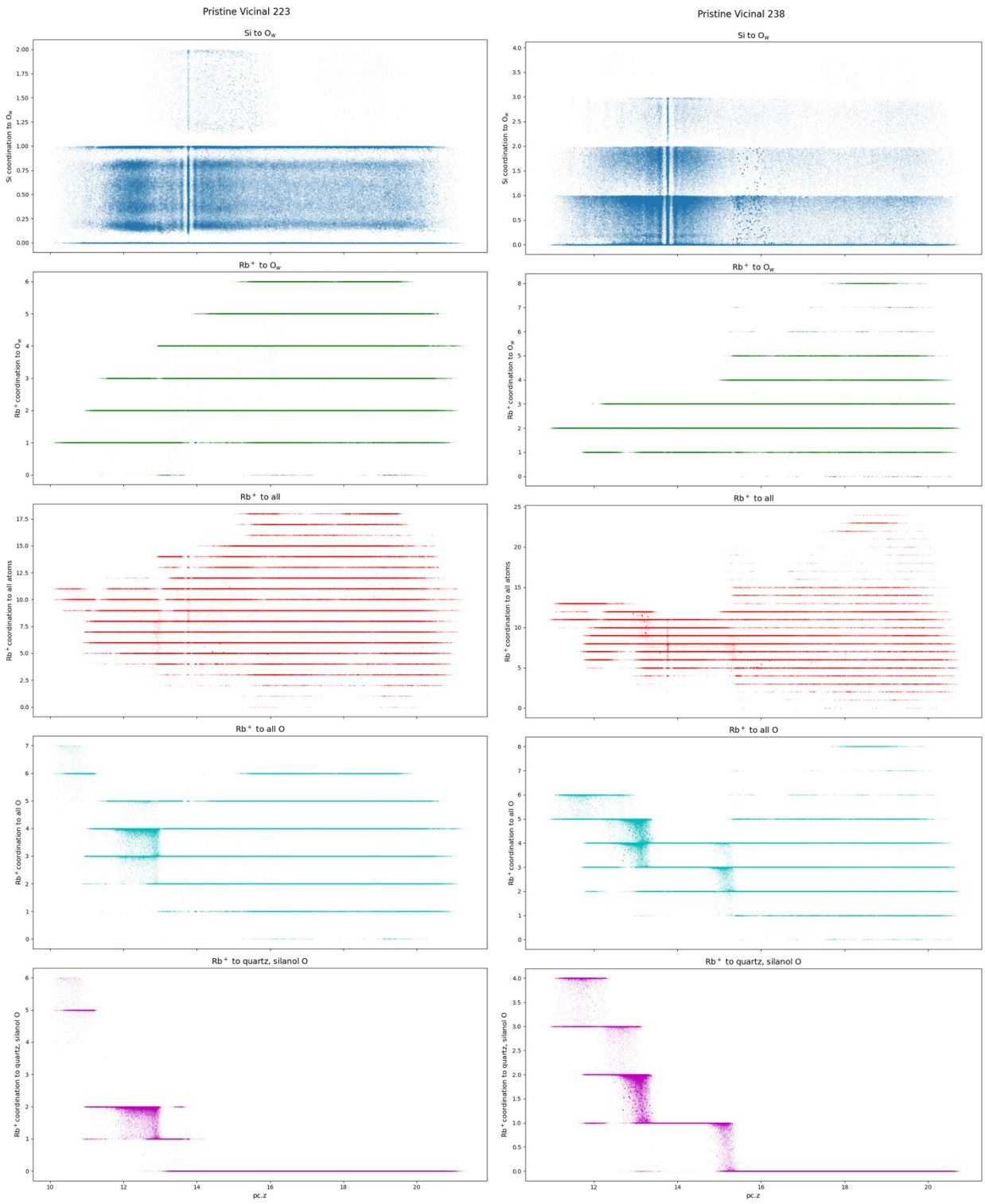

Pristine Vicinal 223
Pristine Vicinal 238
Si to O_w
Si coordination to O_w
Rb^+ to O_w
Rb^+ coordination to O_w
Rb^+ to all
Rb^+ coordination to all atoms
Rb^+ to all O
Rb^+ coordination to all O
Rb^+ to quartz, silanol O
Rb^+ coordination to quartz, silanol O
pc.z

Table S15: Rb^+ coordination to all atoms, water, quartz, and silanol oxygen for defect systems

	Target Position (A)	Coordination Target	Average Position, Å	Si-O to Ow	Rb^+ to Ow	Rb^+ to all	Rb^+ to all O	Rb^+ to Si-O	Frames
Defect Geminal 234	-0.57	0	-0.578	0	3	13.6	6	3	49
	-0.57	1	-0.57	1	3	13.5	6	3	38
	-0.57	2	-0.594	2	3	12.6	6	3	5
	-0.57	All (Distance-Only)	-0.573	0.8	3	13.4	6	3	358
	2.62	0	2.62	0	3	12.8	5	2	2942
	2.62	1	2.62	1	3	12.9	5	2	1064
	2.62	2	2.623	2	3	12.8	5	2	137
	2.62	3	2.625	3	3	12.2	5	2	42
	2.62	All (Distance-Only)	2.62	1	3	12.9	5	2	22920
	5.18	0	5.178	0	1.7	6.4	2.5	0.8	131
	5.18	1	5.18	1	1.8	6.7	2.7	0.9	49
	5.18	2	5.17	2	1.5	6.6	2.5	0.9	19
	5.18	3	5.186	3	1.2	6.2	2.2	1	8
	5.18	All (Distance-Only)	5.178	1.3	1.7	6.8	2.6	0.9	1147
Defect Vacancy 234	2.46	0	2.46	0	3	12.8	5	2	451
	2.46	1	2.467	1	3	12.8	5	2	271
	2.46	2	2.461	2	3	12.8	5	2	83
	2.46	3	2.461	3	3	12.6	5	2	52
	2.46	4	2.461	4	3	12.5	5	2	11
	2.46	All (Distance-Only)	2.46	1.3	3	12.8	5	2	7155
	5.85	0	5.847	0	2	8	3	1	9
	5.85	All (Distance-Only)	5.853	0.1	1.8	7.2	2.7	1	12
Defect Vicinal 217	2	0	2	0	2.6	10.9	4.6	2	2588
	2	1	2	1	2.9	11.8	5	2	681
	2	2	2.005	2	3	12	5	2.1	354

	2	3	2.001	3	3	12.5	5.1	2.1	247
	2	4	2	4	4	16.5	6.3	2.3	43
	2	5	1.979	5	4	16	6	2	2
	2	All (Distance-Only)	2	1.3	3	12.3	5.1	2.1	22372
	4.51	0	4.505	0	3.2	10.3	3.6	0.4	153
	4.51	1	4.509	1	3.9	11.9	4.1	0.2	57
	4.51	2	4.505	2	3.3	9.4	3.3	0	46
	4.51	3	4.519	3	3.7	10.6	3.7	0	27
	4.51	All (Distance-Only)	4.509	1.4	3.5	10.5	3.7	0.1	1851
Defect Vicinal 222	0.77	0	0.768	0	0	6.9	4.8	4.8	893
	0.77	1	0.766	1	0	6.9	4.8	4.8	259
	0.77	All (Distance-Only)	0.769	0.4	0	7	4.9	4.9	2343
	2.72	0	2.721	0	0	2.9	2	2	12204
	2.72	1	2.723	1	0	2.9	2	2	246
	2.72	All (Distance-Only)	2.72	0.1	0	2.9	2	2	14032
	5.05	0	5.048	0	0	1.1	0.4	0.4	1365
	5.05	1	5.05	1	0	0.1	0	0	226
	5.05	All (Distance-Only)	5.048	0.3	0	0.6	0.2	0.2	2654
Defect Vicinal 223	-0.32	0	-0.314	0	1	9.9	5.1	4.1	70
	-0.32	1	-0.313	1	1	10.5	5.5	4.5	11
	-0.32	All (Distance-Only)	-0.314	0.4	1	10.3	5.4	4.4	150
	2.6	0	2.598	0	1	5.2	2	1	2963
	2.6	1	2.6	1	2.2	8.4	3.5	1.3	1030
	2.6	2	2.6	2	2.9	12.3	4.9	1.9	49
	2.6	All (Distance-Only)	2.599	0.4	1.7	7	2.9	1.2	8166
	4.27	0	4.269	0	2.3	7.8	2.8	0.5	70
	4.27	1	4.263	1	2.3	7.9	3	0.6	58
	4.27	2	4.27	2	2.8	9.6	3.5	0.7	10
	4.27	All (Distance-Only)	4.268	0.8	2.4	8.3	3.1	0.7	554

Table S16: Rb^+ coordination to all atoms, water, quartz, and silanol oxygen for pristine systems

	Target Position (A)	Coordination Target	Average Position, Å	Si-O to Ow	Rb^+ to Ow	Rb^+ to all	Rb^+ to all O	Rb^+ to Si-O	Frames
Geminal 234	2.82	0	2.821	0	3	14.8	6	3	3276
	2.82	1	2.819	1	3	14.8	6	3	846
	2.82	2	2.819	2	3	14.8	6	3	766
	2.82	3	2.814	3	3	14.7	6	3	348
	2.82	All (Distance-Only)	2.82	1.1	3	14.8	6	3	26419
	4.85	0	4.845	0	3	10.5	3.7	0.7	167
	4.85	1	4.846	1	3	10.6	3.8	0.8	57
	4.85	2	4.844	2	3	10	3.5	0.6	43
	4.85	All (Distance-Only)	4.844	1	3	10.3	3.6	0.6	1047
Vacancy 234	2.43	0	2.429	0	2.9	13.7	5.9	3	1746
	2.43	1	2.431	1	3	13.7	6	3	1001
	2.43	2	2.432	2	3	13.5	6	3	685
	2.43	3	2.43	3	3	13.1	6	3	375
	2.43	4	2.427	4	3	13	6	3	114
	2.43	All (Distance-Only)	2.43	1.5	3	13.5	6	3	26915
	5.63	0	5.642	0	2.1	6.3	2.1	0	15
	5.63	1	5.628	1	1.9	5	1.9	0	15
	5.63	All (Distance-Only)	5.631	0.9	2.1	5.7	2.1	0	172
Vicinal 217	1.19	0	1.187	0	0.9	6.9	3.6	2.8	260
	1.19	1	1.188	1	0.7	6.7	3.6	2.9	103
	1.19	2	1.196	2	0.6	6.5	3.4	2.8	30
	1.19	3	1.185	3	0.8	5.5	3.3	2.5	18
	1.19	All (Distance-Only)	1.192	0.9	0.8	6.4	3.4	2.7	1927
	2.59	0	2.591	0	1	6.5	2.9	2	3051
	2.59	1	2.588	1	1	6.7	3	2	792

	2.59	2	2.591	2	1.7	8.5	3.6	2	379
	2.59	3	2.591	3	1.9	8.7	3.8	1.9	478
	2.59	All (Distance-Only)	2.59	1.1	1.2	7.3	3.2	2	25336
	4.52	0	4.515	0	2.4	7.7	2.7	0.3	129
	4.52	1	4.524	1	2.2	7.2	2.5	0.3	39
	4.52	2	4.507	2	1.3	3.5	1.3	0	11
	4.52	3	4.542	3	1.4	4.6	1.4	0	5
	4.52	All (Distance-Only)	4.517	0.9	2.4	7.8	2.7	0.4	778
Vicinal 222	1.05	0	1.054	0	1.7	8.5	4	2.3	81
	1.05	1	1.041	1	1.1	6.9	3.7	2.6	35
	1.05	2	1.039	2	1	7.2	4.1	3.1	10
	1.05	All (Distance-Only)	1.047	1.1	1.2	7.4	3.9	2.7	491
	2.87	0	2.871	0	1.4	8.9	4.4	3	4791
	2.87	1	2.871	1	1.5	9.3	4.5	3	919
	2.87	2	2.87	2	1.6	9.4	4.6	3	386
	2.87	3	2.868	3	1.4	8.9	4.3	3	403
	2.87	4	2.874	4	2	10	5	3	45
	2.87	All (Distance-Only)	2.87	1.2	1.5	9.2	4.5	3	31781
	5.32	0	5.322	0	1.3	5.3	2	0.7	50
	5.32	1	5.323	1	1.4	6	2.3	0.9	8
	5.32	2	5.32	2	1.5	5	2	0.5	2
	5.32	All (Distance-Only)	5.32	0.8	1.5	5.9	2.2	0.7	265
Vicinal 238	3.7	0	3.676	0	2.1	8.2	3.1	1	2940
	3.7	1	3.68	1	2.3	8.5	3.3	1	432
	3.7	2	3.684	2	2.1	7.8	3.1	1	103
	3.7	Coordination 3.0	3.679	3	2.2	8.3	3.2	1	23
	3.7	All (Distance-Only)	3.678	0.7	2.2	8.3	3.2	1	8156
	5.21	0	5.207	0	2.3	8.3	3	0.7	922
	5.21	1	5.21	1	2.2	8.3	2.9	0.7	88
	5.21	2	5.202	2	2.9	9.3	3.2	0.3	19
	5.21	3	5.198	3	3.3	10.7	3.6	0.3	6
	5.21	All (Distance-	5.208	0.7	2.3	8.4	3	0.7	2198

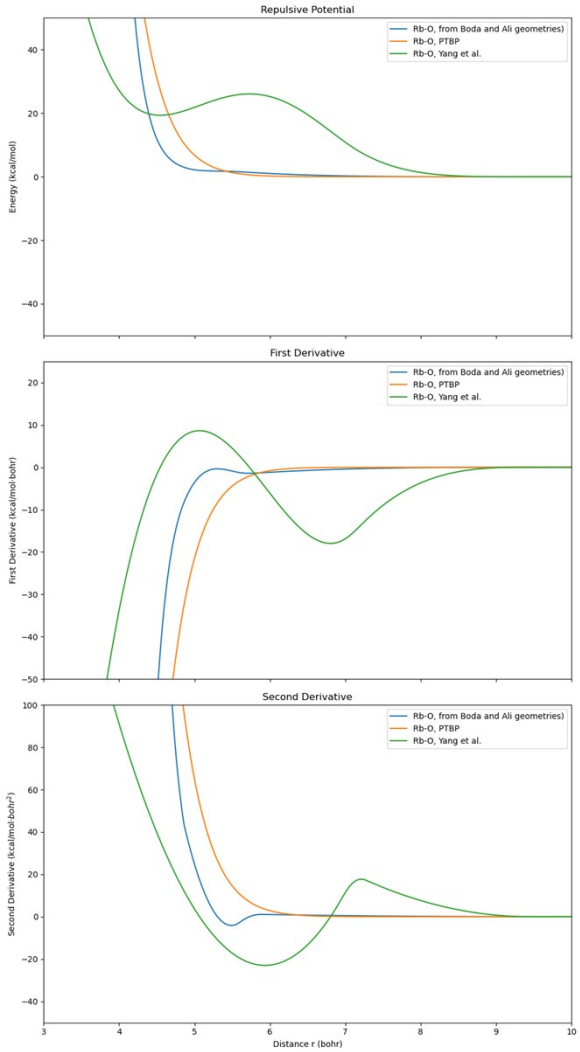
		Only)							

Table S17: Bond lengths for Rb^+ hydrates

The longest Rb-O bond length following geometry optimization starting from Zhu *et al.*[11] coordinates. The Yang *et al.* parameters are assessed at DFTB3, whereas the periodic table baseline parameter set (PTBP) parameters[7] use the corresponding DFTB2. Grimme D3 dispersion[9] is considered for both models.

Hydrate	Yang et al. params	Yang et al. params, D3	0.7x Yang et al. Rb-O spline	Rb-O Spline with Boda and Ali geometries	DFTB2/PTBP	DFTB2-D3/PTBP	Boda and Ali[8] B3LYP/ 6–311++G(d, p)
$Rb(H2O)^+$	2.329	2.329	2.282	2.615	2.881	2.877	2.820(0)
$Rb(H2O)_2^+$	2.327	2.326	2.282	2.612	2.884	2.882	2.839(8)
$Rb(H2O)_3^+$	2.335	2.335	2.318	2.617	2.890	2.888	2.859(3)
$Rb(H2O)_4^+$	2.341	2.274	2.322	2.627	2.914	2.912	2.860(6)
$Rb(H2O)_5^+$	2.361	2.366	2.351	2.617	2.994	2.963	3.085(6)
$Rb(H2O)_6^+$	2.372	2.371	2.365	2.572	2.946	2.936	2.994(8)
$Rb(H2O)_7^+$	2.403	2.400	2.402	2.589	2.990	2.988	3.134(5)
$Rb(H2O)_8^+$	2.419	2.415	2.421	2.600	2.997	2.992	3.270(3)

Figure S6: Spline repulsive potential for original, modified, and PTBP parameters



In Figure S6, the spline repulsive parameters are shown for parameters that best reproduce the geometries of the pentaquo Rb^+ complexes and above, including the PTBP parameters[7] and a potential fitted to the geometries reported by Boda and Ali.[8] We see that those parameters are nearly flat in the repulsive potential, indicating a necessary compromise between representing the solvated Rb^+ case and the Rb^+ to surface silanol interactions captured by the parameter from Yang *et al.*[6]

System coordinates

Coordinates for the pristine and defect surface vicinal 238 systems in xyz format. The surface models are adapted from Yuan *et al.*[12]

Pristine surface simulation box vectors:

0.9942380905E+01	0.0000000000E+00	0.0000000000E+00
0.0000000000E+00	0.1391827965E+02	0.0000000000E+00
0.0000000000E+00	0.0000000000E+00	0.2270000000E+02

Defect surface simulation box vectors:

0.9942299843E+01	0.0000000000E+00	0.0000000000E+00
0.0000000000E+00	0.1391819954E+02	0.0000000000E+00
0.0000000000E+00	0.0000000000E+00	0.2154394228E+02

```
279
Pristine Vicinal 238
O     9.9108229100E+00   1.0299701270E+01   3.4729915000E+00
O     4.8908256000E+00   1.0250202020E+01   3.5445171400E+00
O     2.4944918200E+00   3.3321368200E+00   3.1641054500E+00
O     7.3541993900E+00   3.4789664500E+00   3.6413189900E+00
O     8.8280430100E+00   9.8653544700E+00   1.0649593600E+00
O     4.3828186100E+00   1.0277993930E+01   9.2881465000E-01
O     1.0214446900E+00   3.3333499400E+00   8.1756238000E-01
O     6.8794415700E+00   3.0043621100E+00   1.1349806600E+00
O     7.8893794000E+00   8.5531834400E+00   3.3867372100E+00
O     3.1723484000E+00   8.5244885200E+00   2.6025075200E+00
O     6.7357047000E-01   1.4979053100E+00   2.6465570200E+00
O     5.6597858500E+00   1.5516788100E+00   3.1278976400E+00
O     9.8331878000E-01   7.3337092600E+00   2.2881746600E+00
O     6.1733713300E+00   7.1417559200E+00   1.8747987400E+00
O     3.3699405500E+00   3.0470780000E-01   2.0388636000E+00
O     8.4096688100E+00   1.6859762000E-01   1.8502378900E+00
O     7.3826518500E+00   1.0996289070E+01   2.9716709300E+00
O     2.3162276200E+00   1.0979684880E+01   2.5692014900E+00
O     9.8516870200E+00   4.1385244800E+00   2.9869581000E+00
O     5.0144911300E+00   4.1904277000E+00   2.4658562000E+00
O     7.4175484120E+00   7.2995861430E+00   6.9049198750E+00
O     2.4489891630E+00   7.5855146820E+00   7.4474239760E+00
O     9.7206611850E+00   6.3038743730E-01   6.9935621130E+00
O     4.6973900430E+00   7.4523780800E-01   7.0234606040E+00
O     2.0030648820E+00   7.5914020860E+00   4.7614277170E+00
O     6.0110988980E+00   7.0641431360E+00   4.5378669800E+00
O     3.8353282210E+00   1.5055174810E-01   4.5943483680E+00
O     9.0551483670E+00   5.6367744550E-01   4.5129994410E+00
O     5.6338474000E+00   1.2887457630E+01   3.2332482500E+00
O     5.0085417000E-01   1.2886851670E+01   2.8988648000E+00
O     8.0143543100E+00   5.9884587800E+00   3.3578575100E+00
```

O	3.1680995100E+00	5.9348262300E+00	2.8077360600E+00
O	8.3737196240E+00	1.2500426760E+01	6.2143348630E+00
O	3.2341725320E+00	1.2554185180E+01	6.7319578630E+00
O	1.3058289380E+00	5.5664061900E+00	6.1718538030E+00
O	5.5418927790E+00	5.5087065820E+00	6.7429443190E+00
O	6.1050297780E+00	1.1409256320E+01	5.3766447410E+00
O	1.5944946390E+00	1.1771637950E+01	5.0120981350E+00
O	8.8447071970E+00	4.7433436600E+00	5.4372529210E+00
O	3.9410001850E+00	4.2948105920E+00	4.8764974330E+00
O	9.9280257460E+00	8.0401981790E+00	6.2960508800E+00
O	4.8910812050E+00	8.1051371950E+00	6.5468660610E+00
O	2.1980290460E+00	1.1239473180E+00	6.1479760720E+00
O	7.2864237360E+00	1.0204070570E+00	6.2277226690E+00
O	8.2354059110E+00	1.1732216960E+01	9.9071864350E+00
O	3.0682871950E+00	1.1392824470E+01	9.1953550930E+00
O	2.1693263170E-01	4.8862096220E+00	1.0380139310E+01
O	5.3195456710E+00	4.8649129540E+00	9.3409039730E+00
O	6.4841923520E+00	1.1655012710E+01	7.8905904430E+00
O	9.5725908570E-01	1.1431901010E+01	7.5052124160E+00
O	9.3028048510E+00	5.0876103570E+00	7.9110614070E+00
O	3.5620481980E+00	4.1448450970E+00	7.5921549900E+00
O	8.0619970060E+00	9.9146640030E+00	6.6424810290E+00
O	2.8441008150E+00	9.8640428700E+00	6.5038819400E+00
O	5.8396356000E-01	3.0923209980E+00	6.5701512400E+00
O	5.6266073710E+00	3.0040598210E+00	6.3314145710E+00
O	8.3708610050E-01	1.0036723440E+01	9.9969106840E+00
O	6.4011418590E+00	9.8519608260E+00	9.8384258170E+00
O	3.6466139990E+00	2.7909599640E+00	9.7288604610E+00
O	8.6335266470E+00	3.0436410910E+00	9.2697219600E+00
O	8.8804350990E+00	8.4515973250E+00	8.7332133540E+00
O	3.9524805810E+00	8.9500542810E+00	8.9159108360E+00
O	1.4280279270E+00	1.7016321340E+00	8.7483335270E+00
O	6.3720107950E+00	1.8130962930E+00	8.6218739330E+00
O	5.4511825540E+00	1.2357051830E+01	1.0215026930E+01
O	6.7804939700E-01	1.2703557080E+01	9.6661233380E+00
O	7.7766738510E+00	5.5554918560E+00	9.9701936340E+00
O	2.7576330830E+00	5.3760295760E+00	9.8082176620E+00
O	9.1050531990E+00	8.5502350160E+00	1.1400616560E+01
O	4.8436048150E+00	8.6373525550E+00	1.1417755470E+01
O	2.1955673380E+00	1.3253781330E+00	1.1236543150E+01
O	6.8572874940E+00	2.1865018850E+00	1.1093182110E+01
O	1.0193171250E+00	7.3346762800E+00	9.6682931580E+00
O	6.1270986700E+00	7.3839719720E+00	9.3082445290E+00
O	3.5394206780E+00	1.2620967850E-01	9.1231554120E+00
O	8.3764855290E+00	4.6617410470E-01	9.7478764050E+00
O	9.3530364390E+00	1.3032904490E+01	1.1887748580E+01
O	3.3713324530E+00	1.2803998780E+01	1.1447381120E+01
O	1.3889115890E+00	6.1966614220E+00	1.2204894960E+01
O	5.6711727110E+00	6.1281673730E+00	1.1643004640E+01
O	4.4111657590E+00	8.4143070040E+00	1.9819688930E+01
O	9.1574382860E+00	7.7622186420E+00	1.8608238890E+01
O	6.3711161990E+00	1.3312126370E+01	2.0595936450E+01
O	5.7206367570E+00	1.1497879180E+01	1.6665450140E+01
O	7.3456420030E+00	6.4678787660E+00	1.3826702550E+01
O	3.2874239840E+00	1.1802387080E+01	1.8507797460E+01
O	7.7289742600E+00	7.5417545060E+00	2.2424690470E+01
O	1.5480192730E-01	6.8467770650E+00	1.4588709050E+01

O	2.7535144110E-01	3.1045894750E+00	1.2611022640E+01
O	7.8059227000E+00	9.7006692340E+00	1.6873372030E+01
O	7.6852850500E+00	2.9109647440E+00	1.3556552870E+01
O	5.0805309420E+00	5.3154553810E+00	2.1734652710E+01
O	2.6755689430E+00	6.5139116180E+00	1.8134313660E+01
O	9.5373194090E+00	4.4674084180E+00	1.5927635270E+01
O	9.6485079480E+00	5.4293302590E+00	2.2153317500E+01
O	2.5801584470E+00	5.8174396040E-01	1.8205729140E+01
O	3.9118577280E+00	4.0456164350E+00	1.9298181010E+01
O	3.4099977270E+00	7.0084835350E+00	1.4131904960E+01
O	5.6254454900E+00	1.0285006090E+01	1.3528207670E+01
O	2.9141263000E+00	7.1732816490E+00	2.2052892700E+01
O	6.4594077490E-01	2.1618116040E+00	1.6829742780E+01
O	1.2542799280E+00	3.7634588740E+00	1.9253202790E+01
O	5.1237096560E+00	3.7230166930E+00	1.5519708490E+01
O	9.1685952020E+00	1.3209782700E+01	1.8961384230E+01
O	5.3642819430E+00	5.7411732330E+00	1.7568112950E+01
O	9.0355486300E+00	1.3530510500E+01	2.1779578620E+01
O	3.0533432280E+00	1.0918704380E+01	2.1064760890E+01
O	9.4511505030E+00	1.3063703840E+01	1.6165283230E+01
O	9.6884785490E+00	1.7820403890E+00	2.0194433430E+01
O	6.1727899910E-01	8.9287555430E+00	2.0862724250E+01
O	6.9867705410E+00	1.3844584920E+01	1.3613183590E+01
O	5.7356383340E+00	7.6547648190E+00	1.5738929830E+01
O	8.0550793670E+00	2.2949466540E+00	1.6345564850E+01
O	1.8975406710E+00	9.2205767530E+00	1.7933907030E+01
O	4.8009456050E+00	1.5006400820E+00	1.7140789860E+01
O	1.5548815780E+00	9.0401703180E+00	1.5224718530E+01
O	6.7755098900E+00	7.2511494040E+00	1.9579492200E+01
O	9.1776154150E+00	1.0383978810E+01	1.9025169510E+01
O	2.2679475920E+00	5.0062260360E+00	1.5782256800E+01
O	1.1526639380E+00	6.3328264360E+00	2.0205727950E+01
O	6.7077681280E+00	1.3768337830E+01	1.7901817740E+01
O	3.7612210740E-01	4.9533739720E-01	1.3905182110E+01
O	1.7885341330E+00	1.3243249960E+01	2.0797773490E+01
O	7.8058546340E+00	3.9110638180E+00	2.0400867490E+01
O	3.0393185210E+00	1.5583237750E+00	2.2206764860E+01
O	5.4465200640E+00	2.0644067270E+00	2.0540113800E+01
O	6.4143858210E+00	1.0530005810E+01	1.9473510940E+01
O	8.0754035750E+00	5.3411443330E+00	1.7982407260E+01
Si	8.5719563800E+00	9.8396531300E+00	2.7321170500E+00
Si	3.7294962800E+00	1.0049594480E+01	2.4134954100E+00
Si	1.0386656500E+00	3.0625487700E+00	2.4597784700E+00
Si	6.1611025500E+00	2.9976663300E+00	2.6562233300E+00
Si	1.4251618500E+00	7.1907641210E+00	6.2689308250E+00
Si	5.9998290890E+00	6.9917802090E+00	6.1954504320E+00
Si	3.4725567140E+00	1.1937690560E-01	6.1706319120E+00
Si	8.5951438460E+00	1.7206165630E-01	5.9869527130E+00
Si	6.9883079500E+00	7.2794975500E+00	3.2909706700E+00
Si	2.2905230400E+00	7.3223153300E+00	3.1974067300E+00
Si	9.5534884900E+00	3.4431285000E-01	2.9931874500E+00
Si	4.6358063100E+00	2.6575131000E-01	3.1699758700E+00
Si	6.0255268400E+00	1.1350770340E+01	3.7229456900E+00
Si	1.0474117600E+00	1.1476215670E+01	3.5039554700E+00
Si	8.5065453500E+00	4.5742765600E+00	3.8449554300E+00
Si	3.6217202600E+00	4.4914583400E+00	3.3007280400E+00
Si	6.6775944340E+00	1.1433424590E+01	9.5185149580E+00

Si	1.3329823500E+00	1.1296847850E+01	9.1192185570E+00
Si	8.9233854090E+00	4.5894010570E+00	9.4292012360E+00
Si	3.8366920430E+00	4.3001578840E+00	9.2101490300E+00
Si	7.2349481410E+00	1.1361719800E+01	6.5251934470E+00
Si	2.2002399060E+00	1.1369695190E+01	6.4418135880E+00
Si	7.3175695050E-02	4.6060446200E+00	6.5551819810E+00
Si	4.5717797060E+00	4.2970241430E+00	6.3195039510E+00
Si	8.5373459140E+00	8.4087680610E+00	7.1507260680E+00
Si	3.6565645040E+00	8.6880887810E+00	7.3486378820E+00
Si	1.0580727850E+00	1.6628115890E+00	7.1448454240E+00
Si	6.0381083160E+00	1.6326647430E+00	7.0833230470E+00
Si	9.8700280730E+00	8.5647322170E+00	1.0005917950E+01
Si	5.3087481110E+00	8.6747806920E+00	9.7874866300E+00
Si	2.6795611540E+00	1.4552614650E+00	9.7084348830E+00
Si	7.5768664060E+00	1.8617492950E+00	9.6843753330E+00
Si	9.1352288640E+00	1.3049006430E+01	1.0251001960E+01
Si	3.8785416180E+00	1.2629889010E+01	9.7838239810E+00
Si	1.4046523620E+00	6.0089659470E+00	1.0454322070E+01
Si	6.2429840820E+00	5.9501884090E+00	1.0085083060E+01
H	7.4327700700E+00	2.2094936400E+00	9.3706299000E-01
H	9.3145686780E+00	7.8762893090E+00	1.2090111040E+01
H	5.0634350700E+00	7.7849510140E+00	1.1908560330E+01
H	2.2042593480E+00	4.8134349400E-01	1.1750224710E+01
H	7.1277056060E+00	2.5187557570E+00	1.1980053150E+01
H	1.4090428390E-01	1.3458014740E+01	1.2351674130E+01
H	3.3552226500E+00	1.1869993170E+01	1.1779309970E+01
H	2.2994922380E+00	6.1126488470E+00	1.2526453060E+01
H	6.3081174060E+00	6.2225186050E+00	1.2388211890E+01
H	7.8495951000E-01	6.4601980700E+00	1.9308896500E+00
H	5.1661913600E+00	7.0315572800E+00	1.9500650700E+00
H	2.5301246100E+00	1.3832993130E+01	2.2454359800E+00
H	8.1101201900E+00	1.3216279650E+01	1.5799815900E+00
H	8.0883040900E+00	9.4278856000E+00	5.7799806000E-01
H	3.9967781400E+00	1.0870146680E+01	2.1138034000E-01
H	1.7014364400E+00	2.8520080800E+00	3.5054725000E-01
H	4.3895530440E+00	9.4487770780E+00	1.9942697900E+01
H	6.9066396670E+00	7.1509215780E+00	1.4320173840E+01
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H	3.6052270220E+00	1.1721895130E+01	1.9433642600E+01
H	5.4129242580E-01	7.7067071670E+00	1.5004841230E+01
H	6.2927422180E+00	2.5449090900E+00	2.0540560750E+01
H	8.9655661520E+00	7.2257992030E+00	1.7801738950E+01
H	7.1522726600E+00	7.3542086200E+00	4.5298589000E-01
H	8.2240988120E+00	9.0014962100E+00	1.6319297490E+01
H	5.1291270100E+00	1.1467268450E+01	1.7422019790E+01
H	8.0741116840E+00	6.0426798260E+00	1.4290534840E+01
H	6.2506168450E+00	1.2514536580E+01	2.0117629630E+01
H	7.2337967900E+00	1.3281939060E+01	2.1049863540E+01
H	2.0563735170E+00	6.4823239680E+00	1.8898529640E+01
H	6.4676341690E+00	1.0764562080E+01	1.6816373230E+01
H	6.7123197130E-01	6.6948550990E+00	1.3788040020E+01
H	8.4443811760E+00	6.9121571350E+00	2.2424463570E+01
H	4.9067312900E-01	4.0124192770E+00	1.2708626600E+01
H	2.2413921670E+00	6.7351911240E-02	2.1272406890E+01
H	1.0385050890E+00	2.6687116000E+00	1.2184792560E+01
H	4.8802785050E-01	4.4322904870E+00	1.6325971130E+01
H	5.5715240650E+00	4.9629706450E+00	2.2493509880E+01

H	8.4793149110E+00	9.7894905630E+00	1.7626491870E+01
H	4.3085076720E+00	5.8517643140E+00	2.2022109970E+01
H	2.9087103950E+00	1.3580908880E+01	1.7948006900E+01
H	9.5497422820E+00	5.2317462900E+00	1.5242803300E+01
H	6.6593230140E-02	4.7053869470E+00	5.7666406880E-02
H	4.3396161200E+00	4.3948246740E+00	2.0156125430E+01
H	7.4153909130E+00	2.8221493610E+00	1.4496080680E+01
H	5.1245151160E+00	1.0082274280E+01	1.2779130800E+01
H	3.5069671880E+00	6.6078498020E+00	1.8594494480E+01
H	4.1991054610E+00	7.3586133360E+00	1.4442993070E+01
H	4.2231984490E-01	5.7493981640E+00	2.1506441770E+01
H	8.6678791330E+00	2.8347385570E+00	1.3498430640E+01
H	9.7619144300E+00	2.4026906490E+00	1.6343678290E+01
H	2.3759420190E+00	6.6667544310E+00	2.1375839220E+01
H	2.7039343860E+00	1.1016515610E+01	1.8195173460E+01
H	4.3904567290E+00	3.3050800840E+00	1.8972155970E+01
H	9.7781188550E+00	2.5387074280E-02	1.9165487160E+01
H	5.2891531620E+00	3.9296552670E+00	1.4606781190E+01
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H	5.3138351400E+00	4.5581319380E+00	1.6036620330E+01
H	4.7066809900E+00	5.2498156440E+00	1.8092032310E+01
H	2.1877622430E+00	3.5226092670E+00	1.9221637500E+01
H	7.8768550810E-01	2.8072975690E+00	1.7609404110E+01
H	5.0266427460E+00	1.0598441320E+01	1.4207449980E+01
H	1.3249838420E+00	4.7118521710E+00	1.9569955290E+01
H	7.5811871390E+00	1.4703976220E+00	1.6630634270E+01
H	9.7823283300E+00	1.2198119460E+01	1.6399965610E+01
H	6.2013574710E+00	5.8027051450E+00	1.8107729220E+01
H	8.2466151120E+00	1.3507187670E+01	1.8976156370E+01
H	5.2437984380E-01	2.3633956850E+00	2.0068021990E+01
H	2.4304007000E+00	1.0176313500E+01	2.0844311170E+01
H	1.0601561700E+00	8.7711840340E+00	1.8016704530E+01
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H	7.0184858860E+00	6.8157893530E+00	2.0382929450E+01
H	8.8236715470E-01	8.0366872630E+00	2.0578818710E+01
H	9.5966148800E+00	1.2850482690E+01	2.1414620560E+01
H	3.8359079520E+00	1.2573704890E+00	1.7390195860E+01
H	8.9081901670E+00	2.2461523550E+00	1.9881164280E+01
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H	2.5074725230E+00	1.1724751660E+01	2.1132061080E+01
H	6.2153522050E+00	8.4320638890E+00	1.6036150830E+01
H	7.5816363210E+00	1.3322435360E+01	1.3061470490E+01
H	3.0451270790E+00	4.4424128660E+00	1.5617585910E+01
H	6.8756746200E+00	1.3196616630E+01	1.4285302720E+01
H	2.2757434890E+00	8.4458978430E+00	1.4895409890E+01
H	3.9109631630E-02	8.7454486800E+00	2.1571894170E+01
H	9.5797105380E+00	9.6939951330E+00	1.9536496060E+01
H	8.3347327090E+00	7.6644411630E+00	1.9168469120E+01
H	5.4551511730E+00	7.0916007430E+00	1.6521615250E+01
H	8.9056833560E+00	1.3252959060E+01	1.6879207720E+01
H	9.9178770680E+00	2.4570233160E-04	1.4673081270E+01
H	4.6126028590E-01	6.6158240940E+00	1.9596588270E+01
H	2.6889772460E+00	8.7960819890E+00	1.8261256360E+01
H	6.5296004980E+00	1.3020508430E+01	1.7242898370E+01
H	2.4094021190E+00	5.5003640220E+00	1.6603950280E+01

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H     4.7189419220E+00   2.1781752140E+00   1.6518208440E+01
H     3.7533794040E+00   1.7324895590E+00   2.1583664670E+01
H     2.2587612830E+00   7.5172643120E+00   2.2661412810E+01
H     5.5518742640E+00   1.1096626370E+00   2.0389448440E+01
H     1.8855336740E+00   1.3401541730E+01   1.9876070850E+01
H     9.4663130690E+00   1.1305609940E+01   1.9182081190E+01
H     6.9946704500E+00   4.1321637220E+00   2.0878046490E+01
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H     8.6575857280E+00   4.1245101640E+00   2.0863203580E+01
H     3.2892285290E+00   1.2861232660E+00   3.9281902000E-01
H     4.5409911510E-01   1.4725832490E+00   1.4104999360E+01
H     7.3543811390E+00   1.0713565370E+01   1.9568220460E+01
H     6.2708427660E+00   9.5724984260E+00   1.9373361800E+01
H     8.1826537640E+00   4.7607565750E+00   1.8790456750E+01
H     8.3732540700E+00   4.8833245960E+00   1.7210529530E+01
Rb    5.3500000000E+00   1.2510000000E+01   1.2730829000E+01
O     4.0396558690E+00   1.2907456460E+01   1.4628633210E+01
H     4.8392014800E+00   1.2511098150E+01   1.4896029050E+01
H     4.2877524550E+00   1.3829511500E+01   1.4479894380E+01



273
Defect_Vicinal_238
H     5.7796210000E+00   3.6111210000E+00   2.6758100000E-01
H     8.0516252130E+00   9.9413073160E+00   1.1442647060E+01
H     2.9087237840E+00   9.0545795900E+00   1.1153516230E+01
H     9.5891377140E+00   2.3020789560E+00   1.0867881830E+01
H     5.1700135330E+00   2.8752032650E+00   1.1263255390E+01
H     8.7204202950E+00   1.3393703580E+01   1.2971793570E+01
H     3.7380766350E+00   3.6974869830E+00   1.6664115260E+01
H     8.9491630010E+00   7.2298985190E+00   1.0976217420E+01
H     6.6800800000E-01   8.5505080000E+00   1.8041510000E+00
H     5.6231430000E+00   7.3499960000E+00   1.8312060000E+00
H     4.2780700000E+00   6.3664000000E-01   9.5384100000E-01
H     8.7348730000E+00   1.8604000000E+00   1.4331540000E+00
H     9.2282710000E+00   1.0940427000E+01   4.0658000000E-01
H     4.5346270000E+00   1.0805052000E+01   4.9525200000E-01
H     9.1242200000E-01   3.7910700000E+00   2.4063200000E-01
H     5.7561213020E+00   6.8782231270E+00   1.2486793380E+01
H     4.8830989440E+00   5.4983302110E+00   1.0824188120E+01
H     5.8557512760E-01   5.4141704580E+00   1.0024808940E+01
H     7.5160973100E-01   8.4024542910E+00   1.1804853780E+01
H     2.0806216430E+00   7.2290994080E+00   9.8988189390E+00
H     6.9206339210E+00   7.8011640560E-01   1.6366903390E+01
H     3.9243279430E-01   1.6662779790E+00   1.7708967970E+01
H     4.6591358830E+00   9.1331384040E+00   1.5446562480E+01
H     7.8674932350E+00   6.2558266550E+00   1.8830741960E+01
H     1.3913170950E+00   1.1254901580E+01   1.5927246320E+01
H     5.5025506810E+00   7.2749828740E+00   1.5112238700E+01
H     6.2040214380E+00   1.1763402720E+01   1.2781344220E+01
H     6.6554745610E+00   5.9480051890E+00   1.9782477660E+01
H     6.2560235610E+00   1.2608539070E+01   1.6686769580E+01
H     2.1117704770E+00   1.1707075030E+01   2.0144185710E+01
H     2.3768254040E+00   6.3924520500E+00   2.4986016820E-01
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H	4.5259678900E+00	2.2150539710E+00	2.0557276300E+01
H	3.0197290000E+00	3.0870810000E+00	3.9847200000E-01
H	6.1368067340E+00	2.3202293270E+00	2.0570043270E+01
H	3.3442529550E+00	4.4174017510E+00	2.1245605350E+01
H	8.6585918330E-01	1.2975416310E+00	1.6267542080E+01
H	8.6235123260E-01	2.9820275270E+00	1.9372939010E+01
H	8.0371530250E+00	7.6732327760E+00	2.0502258490E+01
H	4.3913599860E+00	6.4772047910E+00	1.4190513070E+01
H	2.6926580260E+00	6.1087067460E+00	1.4988999470E+01
H	2.7973848690E+00	1.3028326600E+01	1.6899315550E+01
H	5.7385536630E+00	1.1015692340E+01	1.4167375570E+01
H	7.2065051590E+00	1.1634633680E+01	1.6461038100E+01
H	8.1974504320E+00	9.1196826490E+00	2.1458811130E+01
H	4.6250034600E+00	9.0337121550E+00	1.7020265930E+01
H	2.4779380000E+00	1.2012792000E+01	7.0017000000E-02
H	8.3673935020E+00	3.9763192130E-01	1.6271010710E+01
H	7.5802827500E-01	1.2004981850E+01	1.7204566180E+01
H	3.8227527130E+00	1.1254804460E-01	1.7673691240E+01
H	9.1744538430E+00	6.0073946540E+00	1.6884300810E+01
H	4.7561072330E+00	1.3585159290E+01	1.5197547580E+01
H	8.6847926190E+00	1.1703532570E+01	1.8880529420E+01
H	8.8499161200E-01	9.0825618440E+00	1.6059184810E+01
H	8.7828965810E+00	1.0448816520E+01	1.7829163280E+01
H	1.1384520590E+00	8.6907716730E+00	1.4676778430E+01
H	4.5450674950E+00	4.6765735840E+00	1.8536807720E+01
H	4.1112841760E-01	6.6636851670E+00	1.3127101260E+01
H	1.1772075450E+00	1.2992565130E+00	1.2321963350E+01
H	4.8158839490E+00	1.2255579380E+01	1.4451470670E+01
H	4.2744000680E+00	7.7358997530E-01	1.9502269560E+01
H	6.7395305980E+00	2.4980412200E+00	1.8056509660E+01
H	3.2701823020E+00	1.3634501270E+01	2.0176958180E+01
H	3.1907586310E+00	3.7081562380E+00	1.8805433610E+01
H	7.8001027350E+00	5.3547931560E+00	1.6385579680E+01
H	2.3553520990E+00	5.1512421230E+00	1.3617512840E+01
H	8.8122366710E+00	2.7040428390E+00	1.9431588090E+01
H	9.0498758690E+00	7.6123450440E+00	1.3237286550E+01
H	9.6631758890E+00	5.0609258240E+00	2.0402164960E+01
H	1.7374743470E+00	1.7354622410E+00	1.9545798530E+01
H	7.8875801030E+00	3.9116419470E+00	1.9520376990E+01
H	5.1735810230E+00	2.4128271060E+00	1.7493168520E+01
H	3.3891457020E+00	1.0047726720E+01	1.3277783100E+01
H	5.6675548610E+00	1.3226192160E+01	2.0713781020E+01
H	1.3263549790E+00	3.9578050440E-01	1.3496042330E+01
H	2.5923386420E+00	9.7553497430E+00	1.4577268000E+01
H	6.9352936990E+00	9.6830060420E+00	1.9730606890E+01
H	3.9990706280E+00	6.2700750450E+00	1.9733858070E+01
H	1.6717845610E+00	5.5853536260E+00	2.0588817770E+01
H	3.9163753480E-01	4.3614185950E+00	1.3938083920E+01
H	8.8021152740E+00	1.1877301840E+01	1.4387438370E+01
H	1.3102141810E+00	6.7505065050E+00	1.6729447020E+01
H	3.3043585220E+00	9.3420999100E+00	1.8749567270E+01
H	7.5941032160E+00	1.5222740550E-01	1.8624423630E+01
H	5.2279930000E+00	1.1792256000E+01	2.0316303000E+01
H	5.0694000210E+00	6.8932808410E+00	1.8777274060E+01
H	7.0809597420E+00	9.2835332290E+00	1.6765213200E+01
H	5.9851280830E+00	5.0894788000E+00	1.5115501410E+01
H	6.1932786630E+00	1.0559579340E+01	1.8615696680E+01

H	8.7212590260E+00	1.2254392110E+01	1.5891456490E+01
H	1.3526393850E+00	9.5242759590E+00	1.8857817910E+01
H	5.6569521190E-01	3.9574969790E+00	1.2477022300E+01
H	1.5220606320E-01	1.2497397520E+01	2.0689351780E+01
H	9.3681037960E+00	8.5278162730E+00	1.9493523260E+01
H	3.0801699530E+00	6.1294953230E-01	1.5280279520E+01
H	6.2318431170E+00	3.6440014330E+00	1.5796379770E+01
H	4.8157030250E+00	9.2322222520E+00	1.9201373180E+01
H	8.0078955020E+00	8.0075077600E+00	1.7127313360E+01
H	8.5191486490E+00	1.2997101490E+01	2.0155514870E+01
H	2.6767735460E+00	7.4686464960E+00	1.7161721640E+01
H	6.8976985810E-01	5.0990353370E+00	1.8850826210E+01
H	1.3144473250E-01	7.6269541500E+00	1.8350009420E+01
H	1.9335388110E+00	1.0940878390E+01	1.8066282690E+01
H	1.0320352930E+00	4.6027542990E+00	1.7427373120E+01
H	8.4115988940E+00	3.8963724740E+00	1.5016503620E+01
H	2.7153252490E+00	1.9890116600E+00	1.5321535810E+01
H	7.3904188560E+00	1.1605946770E+00	1.9779829380E+01
H	9.4101893760E+00	3.0063728090E+00	1.5814360670E+01
H	3.2581623670E+00	4.0518889420E+00	1.5136325630E+01
H	4.2992767850E+00	1.3727155160E+01	8.0341567980E+00
H	3.2783163250E+00	1.3091913520E+01	9.8752349350E+00
H	3.4446766530E+00	1.4720119780E+00	9.7469220420E+00
O	2.3393840920E-01	1.0805070400E+01	3.2047385850E+00
O	5.2423790000E+00	1.0815155000E+01	3.2060740000E+00
O	2.7570130000E+00	3.8559610000E+00	3.2059230000E+00
O	7.7282040000E+00	3.8559610000E+00	3.2059230000E+00
O	8.8483040000E+00	1.0275578000E+01	9.5957700000E-01
O	3.8771130000E+00	1.0275578000E+01	9.5957700000E-01
O	1.3915530000E+00	3.3164090000E+00	9.5954800000E-01
O	6.3627410000E+00	3.3164100000E+00	9.5954800000E-01
O	8.2781560000E+00	9.0675250000E+00	3.2477670000E+00
O	3.3069660000E+00	9.0675250000E+00	3.2477670000E+00
O	8.2152100000E-01	2.1084050000E+00	3.2478230000E+00
O	5.7927110000E+00	2.1084050000E+00	3.2478230000E+00
O	1.3917670000E+00	7.9292320000E+00	1.7549760000E+00
O	6.3629570000E+00	7.9292320000E+00	1.7549760000E+00
O	3.8773240000E+00	9.7028600000E-01	1.7550560000E+00
O	8.8485150000E+00	9.7028600000E-01	1.7550560000E+00
O	7.7279620000E+00	1.1672455000E+01	2.8910480000E+00
O	2.7567720000E+00	1.1672455000E+01	2.8910480000E+00
O	2.7139500000E-01	4.7133730000E+00	2.8911160000E+00
O	5.2425850000E+00	4.7133730000E+00	2.8911160000E+00
O	7.7276560000E+00	8.1386100000E+00	6.5888970000E+00
O	2.6178318090E+00	8.3204348470E+00	6.6415574550E+00
O	3.2041890030E-01	1.1605890370E+00	6.4002120910E+00
O	5.2249919460E+00	1.2813097110E+00	6.6167130530E+00
O	1.3963191420E+00	7.4397924250E+00	4.3542169180E+00
O	6.4133300810E+00	7.6149709120E+00	4.4367842010E+00
O	3.8348988780E+00	9.3889806530E-01	4.3003738490E+00
O	8.8443902400E+00	6.0401290490E-01	4.3039674670E+00
O	5.6958019280E+00	1.3359408430E+01	2.8373398760E+00
O	8.2149900000E-01	1.3420102000E+01	2.8495070000E+00
O	8.2783930000E+00	6.4609810000E+00	2.8495010000E+00
O	3.3072020000E+00	6.4609810000E+00	2.8495010000E+00
O	8.2780510000E+00	1.3350068000E+01	6.6303430000E+00
O	3.4186525390E+00	1.3496665240E+01	6.5320184070E+00

O	8.1611072460E-01	6.4127704700E+00	6.7107060590E+00
O	5.5949597850E+00	6.5357388470E+00	6.6997286710E+00
O	6.4409965530E+00	1.2330306030E+01	5.1839277490E+00
O	1.4411693310E+00	1.2173578960E+01	5.1714747870E+00
O	8.8417122680E+00	5.3120215110E+00	5.1182905480E+00
O	4.0797073430E+00	5.1656481930E+00	5.1284025680E+00
O	1.2321576170E-01	8.9242620590E+00	6.0929477510E+00
O	5.1157161180E+00	9.1943660740E+00	6.2217255630E+00
O	2.7517846600E+00	2.0600681890E+00	6.6080625390E+00
O	7.7378456840E+00	1.9268512340E+00	6.2686779730E+00
O	7.0728007640E+00	1.3199866590E+01	1.0069309850E+01
O	2.3398221110E+00	1.3233065150E+01	1.0108940380E+01
O	9.7334505490E+00	6.0220593200E+00	9.9064200660E+00
O	4.4480453430E+00	4.7701660800E+00	1.0297124280E+01
O	6.2558067270E+00	1.1969751460E+01	7.8168748140E+00
O	1.3039331830E+00	1.2506344890E+01	7.7541724320E+00
O	8.8323491830E+00	4.8510324030E+00	7.6950305840E+00
O	3.6972047310E+00	5.0996447450E+00	7.7589711860E+00
O	8.2722370280E+00	1.0747173110E+01	6.7427133400E+00
O	3.2927284250E+00	1.0975244330E+01	6.7621794540E+00
O	8.7438912340E-01	3.8195779260E+00	6.3670194670E+00
O	5.8791769040E+00	3.8994489780E+00	6.6981083210E+00
O	1.0660098900E+00	1.0833616340E+01	9.7376256870E+00
O	5.2253229170E+00	1.1326956410E+01	1.0092178530E+01
O	1.9029658620E+00	4.4092512530E+00	9.6784636820E+00
O	7.8754226130E+00	4.0292628680E+00	1.0014585410E+01
O	9.2947028250E+00	9.1053521330E+00	8.6356008610E+00
O	4.0201206400E+00	9.3437083680E+00	8.6668236180E+00
O	1.0358173850E+00	2.1304295630E+00	8.5987186400E+00
O	6.4844201660E+00	2.2999300870E+00	8.6037763790E+00
O	4.7252970090E+00	1.3690956170E+01	8.9273723950E+00
O	9.7518113430E+00	1.3131311880E+01	1.0165632180E+01
O	7.1285705750E+00	6.4534788720E+00	9.2540859050E+00
O	2.9253650580E+00	6.8991685990E+00	9.4646994350E+00
O	8.7052818470E+00	1.0364311540E+01	1.0846722970E+01
O	3.7260348650E+00	9.5897740110E+00	1.1286286280E+01
O	4.5301262640E-01	2.8153829780E+00	1.1167782240E+01
O	6.0673771700E+00	2.5750593850E+00	1.1302017030E+01
O	7.6272794590E-01	8.4613360520E+00	1.0840326690E+01
O	6.2079094410E+00	8.9302907660E+00	1.0191125290E+01
O	3.0050424590E+00	2.0196151210E+00	1.0447947070E+01
O	8.2773746020E+00	1.4540356260E+00	1.0500490950E+01
O	8.0583344820E+00	1.3477728530E+01	1.2312151020E+01
O	3.4482525620E+00	3.3689745080E+00	1.5770338800E+01
O	8.1418530880E+00	7.6369930220E+00	1.1383828080E+01
O	5.6308919610E+00	6.7083346870E+00	1.1522596670E+01
O	3.7644712930E+00	3.5256063440E+00	2.1460160400E+01
O	5.3207360510E+00	6.6771526300E+00	1.4367547490E+01
O	6.4302410520E+00	1.1161729150E+01	1.3473254090E+01
O	6.2645806010E+00	1.1727148810E+01	1.6290752000E+01
O	2.5444957830E+00	5.9849521250E+00	2.0907084470E+01
O	5.3773503920E+00	1.7265085080E+00	2.0440381830E+01
O	1.6832964490E-02	1.5030922980E+00	1.6769949530E+01
O	7.6202323360E+00	6.0692497510E+00	1.9725439370E+01
O	1.9453511390E+00	1.2309791860E+01	2.0829786580E+01
O	5.2206116620E+00	8.8688450190E+00	1.6249127530E+01
O	7.5496408380E+00	1.8022259640E-01	1.6717111480E+01

O	3.6512229490E+00	1.3551149140E+01	1.6846444140E+01
O	1.5612478100E+00	1.1756087380E+01	1.6743199830E+01
O	7.9893270830E+00	8.6582539720E+00	2.0609905400E+01
O	4.0436931960E+00	3.8126739810E+00	1.8337246510E+01
O	8.7838872870E+00	1.1440847820E+01	1.7921987640E+01
O	3.3854893770E+00	3.2272822790E-01	1.9433130610E+01
O	4.7238854700E+00	1.3182882260E+01	1.4295726350E+01
O	8.9035711010E-01	9.4788044600E+00	1.5212313310E+01
O	8.1963052000E+00	5.9225547480E+00	1.7074433230E+01
O	6.9760325460E-01	6.8713717100E-01	1.2873812560E+01
O	7.3030544240E-02	7.5587759800E+00	1.3259713540E+01
O	1.3936792730E+00	2.3383315930E+00	1.8875816410E+01
O	3.4798147450E+00	9.8395803760E+00	1.4183404930E+01
O	6.1182660730E+00	2.4136928880E+00	1.7282269130E+01
O	2.9436832260E+00	5.7727291880E+00	1.4113995870E+01
O	7.8458864430E+00	2.9059861730E+00	1.9396600780E+01
O	4.8302495890E-01	4.5440845080E+00	2.0208935590E+01
O	4.8971567790E+00	6.1655111580E+00	1.9354579990E+01
O	6.0986277040E+00	1.0177617300E+01	1.9487287680E+01
O	5.1036946830E+00	1.2487629470E+01	2.0943653080E+01
O	9.1669811350E+00	1.2451467720E+01	1.5072640410E+01
O	4.1175660100E+00	8.7646331950E+00	1.8653813650E+01
O	7.1570831750E-01	4.7151483940E+00	1.3088545510E+01
O	2.1972948120E-01	8.2913243130E+00	1.9017114540E+01
O	2.3705934020E+00	1.1405626520E+00	1.4983833130E+01
O	9.1491505350E+00	1.2255472920E+01	2.0403902720E+01
O	2.0925599860E+00	7.2911678570E+00	1.6359405070E+01
O	9.3698748540E-01	5.4351759650E+00	1.7904769930E+01
O	7.5252711360E+00	1.5956837670E-01	1.9613941280E+01
O	2.0082940910E+00	1.0279707280E+01	1.8833222960E+01
O	7.8572449830E+00	8.9589267770E+00	1.7218974400E+01
O	9.3416609350E+00	3.8279125040E+00	1.5227891640E+01
O	6.6194598390E+00	4.5174212530E+00	1.5553090880E+01
Si	8.7873259130E+00	1.0490580880E+01	2.6130031540E+00
Si	3.7925630000E+00	1.0459603000E+01	2.5730040000E+00
Si	1.3071320000E+00	3.5004580000E+00	2.5729630000E+00
Si	6.2783230000E+00	3.5004580000E+00	2.5729630000E+00
Si	1.3068150000E+00	7.7829840000E+00	5.9555100000E+00
Si	6.1923228630E+00	7.9142845850E+00	6.0187957810E+00
Si	3.7949937570E+00	9.9906244850E-01	5.9102506350E+00
Si	8.7801929900E+00	7.4740078440E-01	5.9232284810E+00
Si	7.3300200530E+00	7.7707555470E+00	3.0769193230E+00
Si	2.3550080000E+00	7.7641620000E+00	3.0486270000E+00
Si	9.8118240000E+00	8.0511700000E-01	3.0486970000E+00
Si	4.8406350000E+00	8.0511700000E-01	3.0486970000E+00
Si	6.2781990000E+00	1.2027973000E+01	3.5242220000E+00
Si	1.3070080000E+00	1.2027973000E+01	3.5242220000E+00
Si	8.7639220000E+00	5.0688220000E+00	3.5241680000E+00
Si	3.7927300000E+00	5.0688220000E+00	3.5241680000E+00
Si	5.8688020000E+00	1.2524349000E+01	9.2841140000E+00
Si	1.0473189640E+00	1.2459872390E+01	9.3938983030E+00
Si	8.3472363790E+00	5.3652683050E+00	9.1624312240E+00
Si	3.2258039670E+00	5.3261493720E+00	9.2951351170E+00
Si	7.3171203460E+00	1.2077804600E+01	6.5287243720E+00
Si	2.3126890810E+00	1.2276737360E+01	6.5421743280E+00
Si	9.7861184180E+00	5.1353432000E+00	6.4452622760E+00
Si	4.8034924330E+00	5.1244680200E+00	6.5446173750E+00

Si	8.8376638560E+00	9.2560367930E+00	7.0816943140E+00
Si	3.7724991760E+00	9.4590953680E+00	7.0870371440E+00
Si	1.2486481840E+00	2.4139791070E+00	7.0324391950E+00
Si	6.4131408830E+00	2.3400683950E+00	7.0158158030E+00
Si	9.9212640180E+00	9.6814939640E+00	1.0039751110E+01
Si	4.8126810820E+00	9.7510836860E+00	1.0015326360E+01
Si	1.6296437540E+00	2.7848409230E+00	9.9279097470E+00
Si	7.1528686100E+00	2.5960298440E+00	1.0035577770E+01
Si	8.3768686980E+00	1.3751654410E+01	1.0676179900E+01
Si	6.7549131160E+00	7.4375364550E+00	1.0523941960E+01
Rb	7.0000000000E+00	1.3200000000E+01	1.4592829000E+01
H	8.8775847850E+00	7.3459970530E-01	1.4185493620E+01
H	7.8945628300E+00	1.0455094360E+00	1.3284882880E+01
O	8.0805219120E+00	1.2089610120E+00	1.4204789760E+01

MetadynMiner scripts

NEB_calcaulations.R

```
library(metadynminer)
library(viridis)
library(colorspace)
plasma_palette <- plasma(84)[84:1]
last_color <- plasma_palette[1]
white_to_last <-
colorRampPalette(c("#FFFFFF",
last_color))(16)
combined_palette <-
c(white_to_last, plasma_palette)
combined_palette[100] <-
darken(plasma_palette[84], amount =
0.6)

data_base_path <- "/
Plumed_Runs_Pristine"
output_base_path <- "
/Plumed_Runs_Pristine/"

#simName <- "Geminal_234"
#simName <- "Vacancy_234"
#simName <- "Vicinal_217"
#simName <- "Vicinal_222"
#simName <- "Vicinal_223"
simName <- "Vicinal_238"

edHills <-
file.path(data_base_path, simName,
"walkers/Combined_HILLS_finalized")
origHills <-
file.path(data_base_path, simName,
"walkers/Combined_HILLS_temp")
pngFesEd <-
file.path(output_base_path,
paste0(simName, "NEB.png"))
pngFesOrig <-
file.path(output_base_path,
paste0(simName,
"_NEB_Original_CV.png"))
pngFesEdProf <-
file.path(output_base_path,
paste0(simName, "_NEB_Prof.png"))
pngFesOrigProf <-
file.path(output_base_path,
paste0(simName,
"_NEB_Original_CV_Prof.png"))

textfile <-
file.path(output_base_path,
paste0(simName, "_NEB.txt"))
sink(textfile, append = T)

hillsf<-read.hills(origHills)
tfes<-fes(hillsf)
minima<-fesminima(tfes)
nebAD<-neb(minima, min1="B",
min2="E", nbins = 20, nsteps =
20000, step = 1, k = 0.3)
print(nebAD[["path"]][["pathx"]])
print(nebAD[["path"]][["pathy"]])
print(nebAD[["path"]][["fespot"]])
png(file=pngFesEd, width=8.5,
height=7.15, units="in", res=1200)
plot(minima)
linesonfes(nebAD)
dev.off()
sink()
```

Plotting_Metadynminer.R

```
library(metadynminer)
library(viridis)
library(colorspace)
plasma_palette <- plasma(84)[84:1]
last_color <- plasma_palette[1]
white_to_last <-
colorRampPalette(c("#FFFFFF",
last_color))(16)
combined_palette <-
c(white_to_last, plasma_palette)
combined_palette[100] <-
darken(plasma_palette[84], amount =
0.6)

data_base_path <- "
/Plumed_Runs_Defect"
output_base_path <- "
/Plumed_Runs_Defect/"

simName <- "Geminal_234"

edHills <-
file.path(data_base_path, simName,
"walkers/Combined_HILLS_finalized")
origHills <-
file.path(data_base_path, simName,
"walkers/Combined_HILLS_temp")
pngFesEd <-
```

```
file.path(output_base_path,
paste0(simName, ".png"))
pngFesOrig <-
file.path(output_base_path,
paste0(simName,
"_Original_CV.png"))
pngFesEdProf <-
file.path(output_base_path,
paste0(simName, "_Prof.png"))
pngFesOrigProf <-
file.path(output_base_path,
paste0(simName,
"_Original_CV_Prof.png"))

textfile <-
file.path(output_base_path,
paste0(simName, ".txt"))

sink(textfile, append = T)
hillsf<-read.hills(edHills)
tfes<-fes(hillsf)
minima<-fesminima(tfes)
png(file=pngFesEd, width=8.5,
height=7.15, units="in", res=1200)
plot(minima, axes=T, xlab = 'Rb(I)
distance from surface, Å',
ylab=expression("O"["SiOH"]*" -
O"["w"]*"  CN"), col =
combined_palette, colscale = T,
textcol="#9FC3E9",nlevels = 10,
colscalelab=expression("Free
energy, kJ·mol"^"-1"), lwd=0.5)
dev.off()
print(minima)
tfes1<-fes2d21d(hillsf, remdim=2)
minima1<-fesminima(tfes1)
png(file=pngFesEdProf, width=8.5,
height=7.15, units="in", res=1200)
plot(minima1, axes=T, xlab = 'Rb(I)
distance from surface, Å',
ylab=expression("Free energy,
kJ·mol"^"-1"))
dev.off()
print(minima1)
hillsf<-read.hills(origHills)
tfes<-fes(hillsf)
minima<-fesminima(tfes)
png(file=pngFesOrig, width=8.5,
height=7.15, units="in", res=1200)
plot(minima, axes=T, xlab = 'Rb(I)
distance from surface, Å',
ylab=expression("O"["SiOH"]*" -
O"["w"]*"  CN"), col =
combined_palette, colscale = T,
textcol="#9FC3E9",nlevels = 10,
colscalelab=expression("Free
energy, kJ·mol"^"-1"), lwd=0.5)
dev.off()
print(minima)
tfes1<-fes2d21d(hillsf, remdim=2)
minima1<-fesminima(tfes1)
png(file=pngFesOrigProf, width=8.5,
height=7.15, units="in", res=1200)
plot(minima1, axes=T, xlab = 'Rb(I)
distance from surface, Å',
ylab=expression("Free energy,
kJ·mol"^"-1"))
dev.off()
print(minima1)
sink()
```

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