Electronic Supplementary information for:

The Interaction of Pu(IV) with Low Index Ferrihydrite Surfaces: A Periodic Boundary Condition DFT Study

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Supplementary Figures

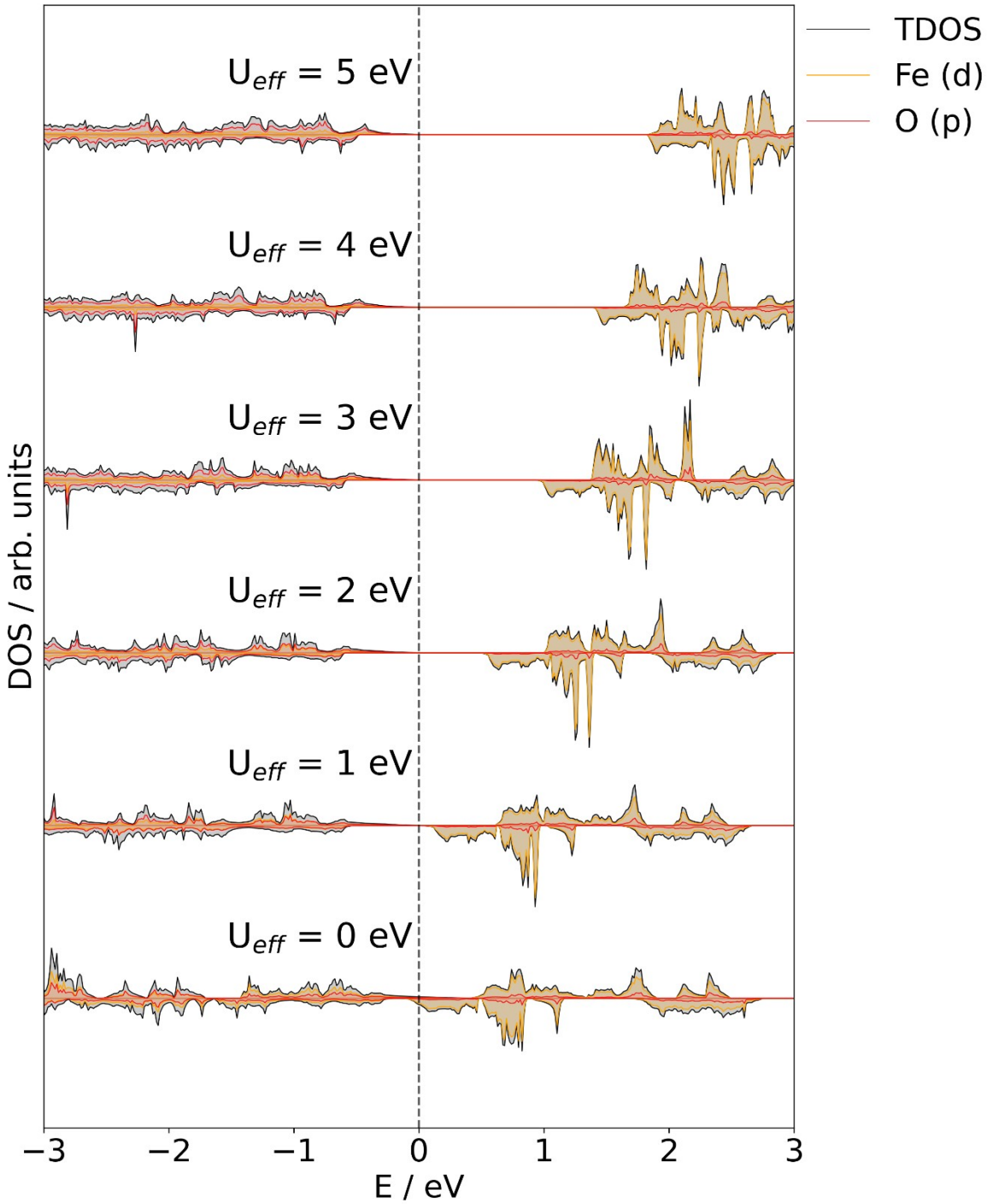

Figure S1: The effect of U_{eff} on the bulk Fe(d) and O(p) density of states. E = 0 eV represents the valence band maximum.

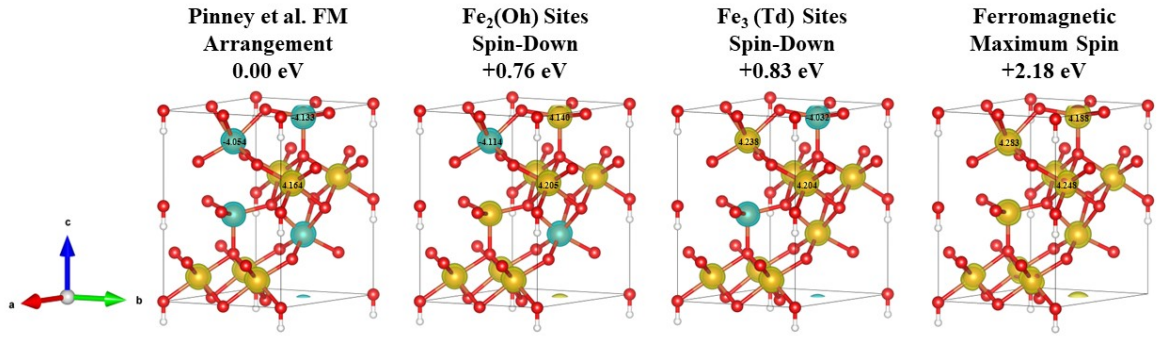

Figure S2: Relative energies between different ferrimagnetic spin arrangements and the ferromagnetic spin arrangement. Energies are presented relative to the lowest energy structure, in agreement with Pinney et al.'s more extensive study regarding bulk Fh magnetism. Colour scheme: Fe, orange; O, red; H, white. Spin-up and spin-down densities are yellow and blue respectively. Magnetic moments for the Fe(d) states are presented on Fe_1(Oh), Fe_2(Oh), and Fe_3(Td) and are equal for symmetrically equivalent Fe atoms (see table S3)

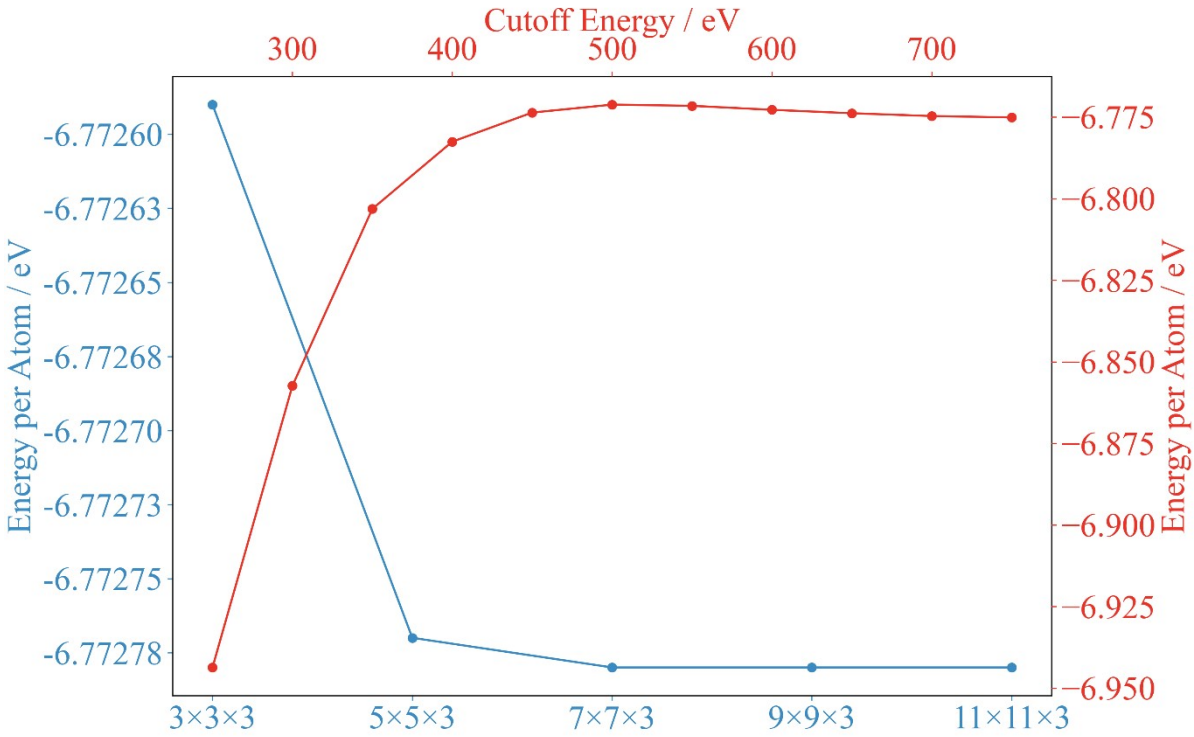

Figure S3: Convergence behaviour of the Fh bulk with respect to ***k***-point sampling and plane wave cutoff energy.

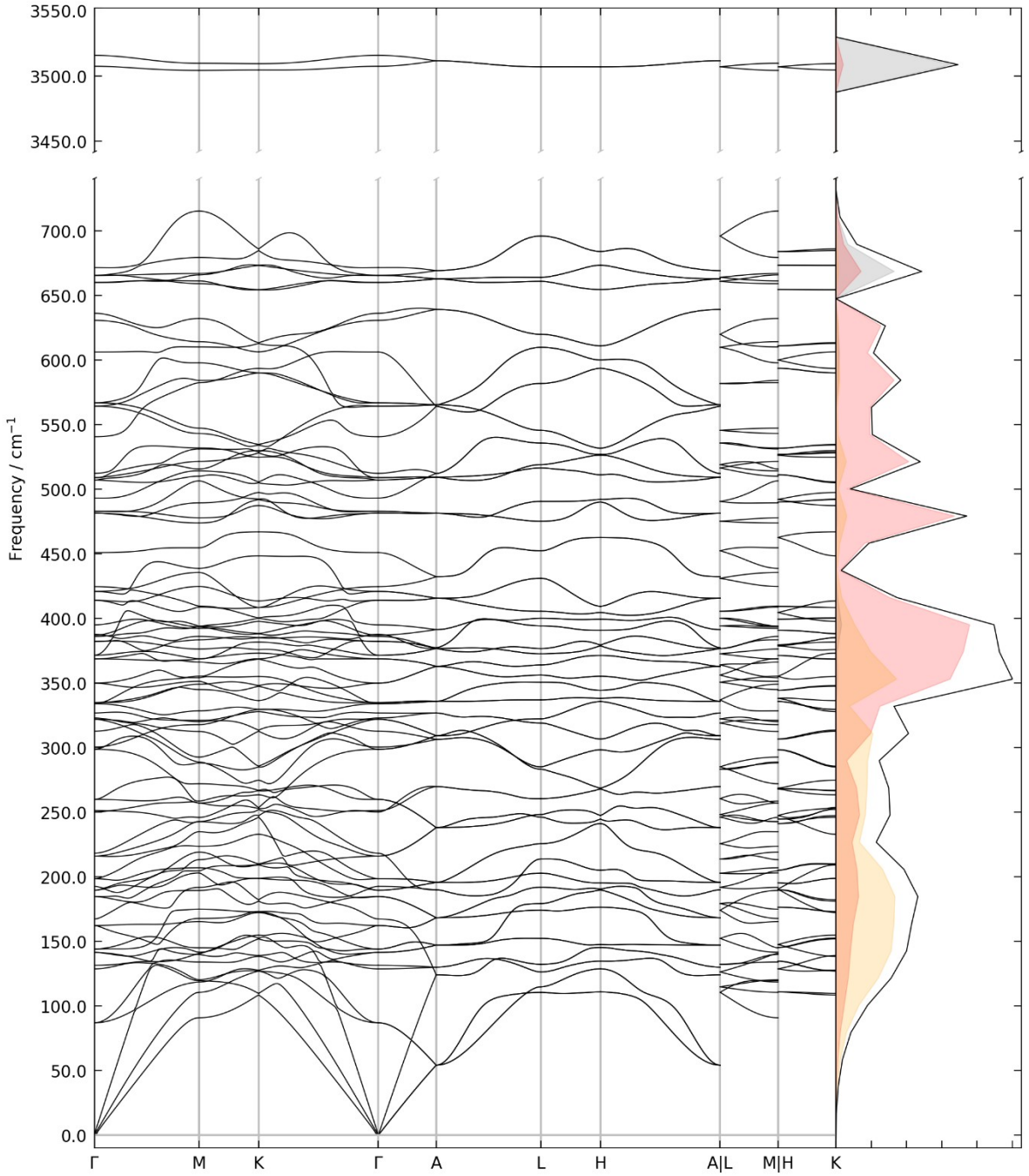

Figure S4: Phonon band structure and projected density of states calculated for the 3 × 3 × 1 supercell expansion of the relaxed Fh bulk unit cell. Colour scheme: Fe, orange; O, red; H, grey.

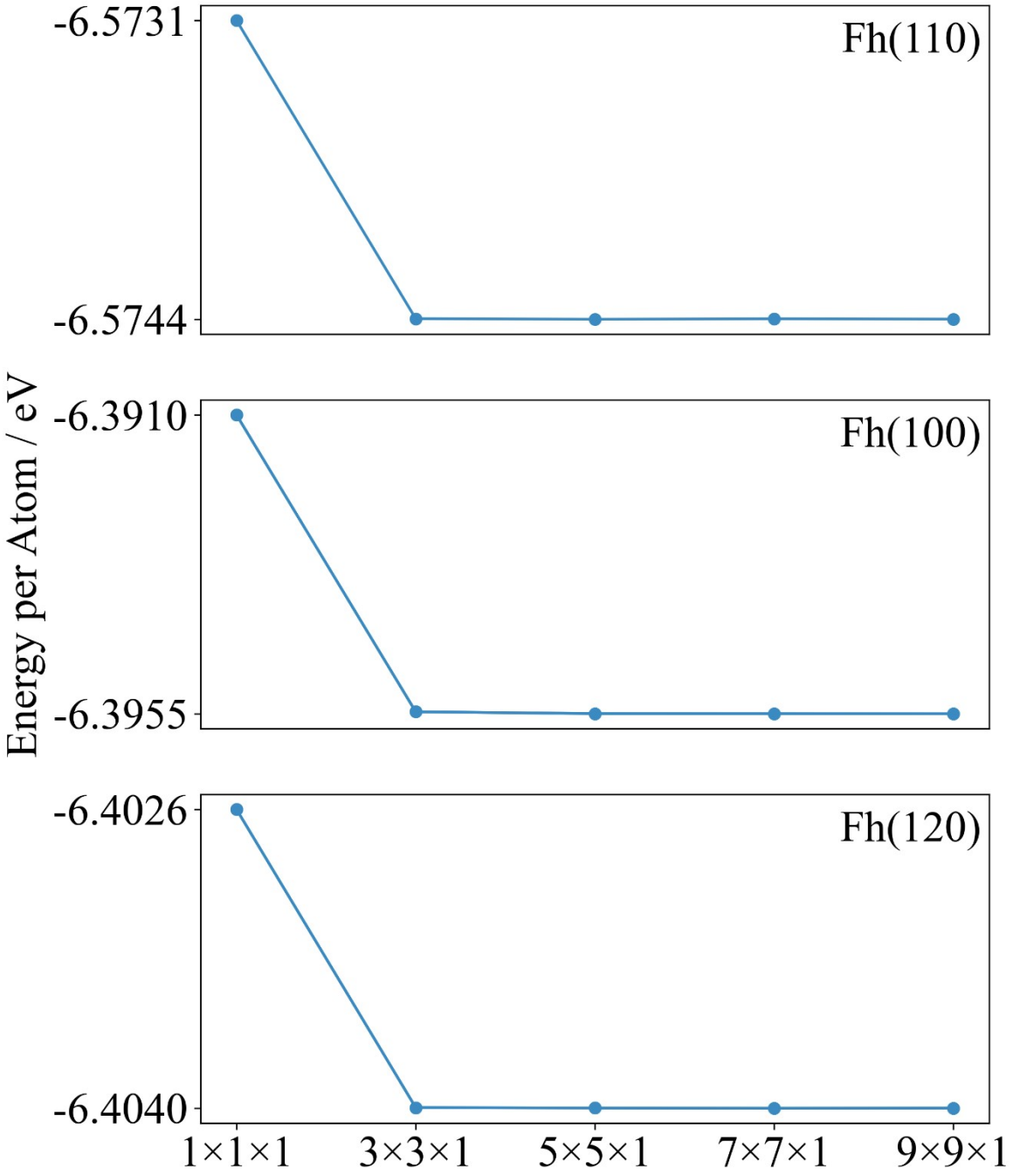

Figure S5: Convergence behaviour of the Fh surfaces with respect to ***k***-point sampling and fixed plane wave cutoff energy of 600 eV.

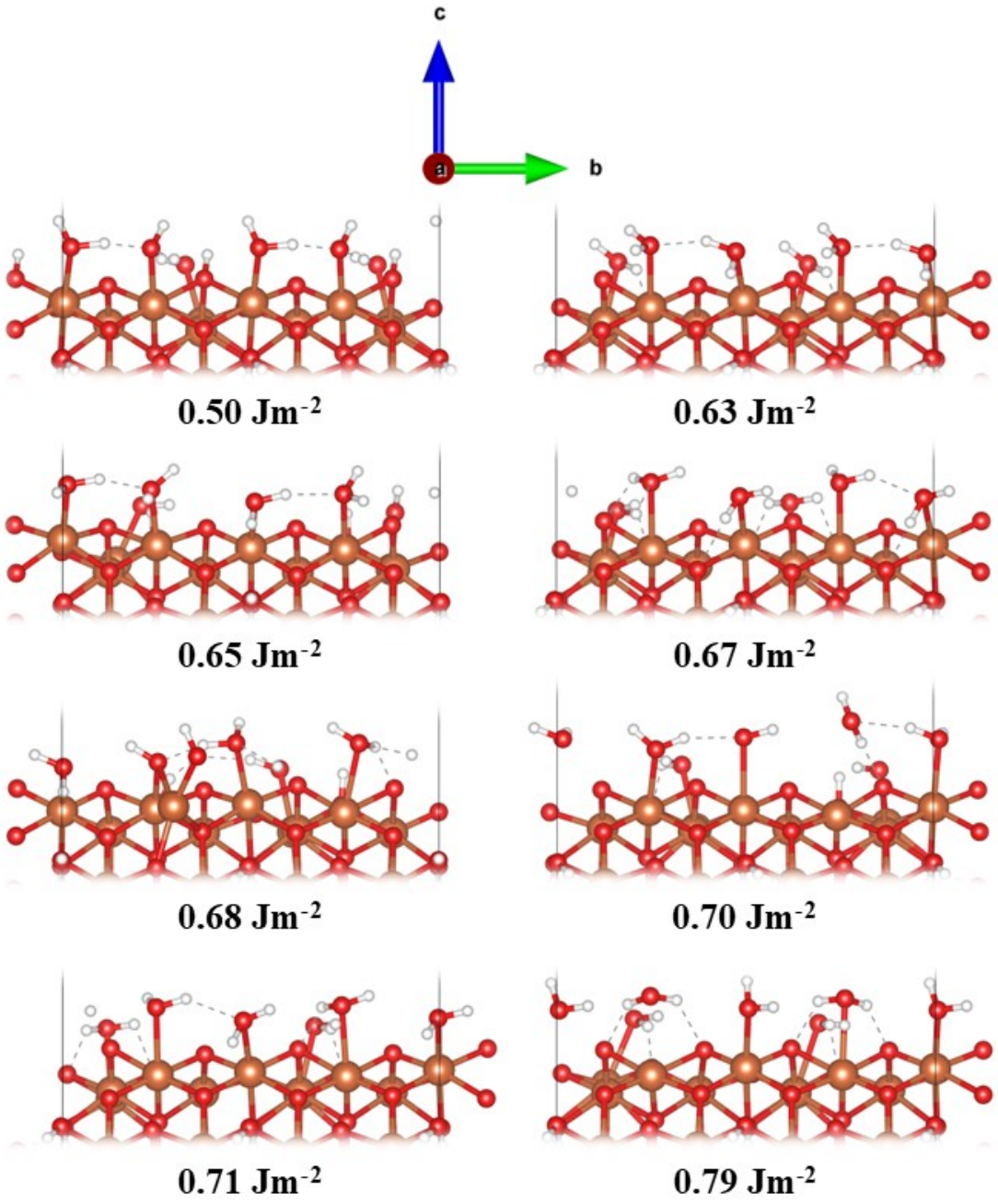

Figure S6: Hydrated Fh(100) surfaces and their corresponding γ_{hydr} surface energies. Colour scheme: Fe, orange; O, red; H, white.

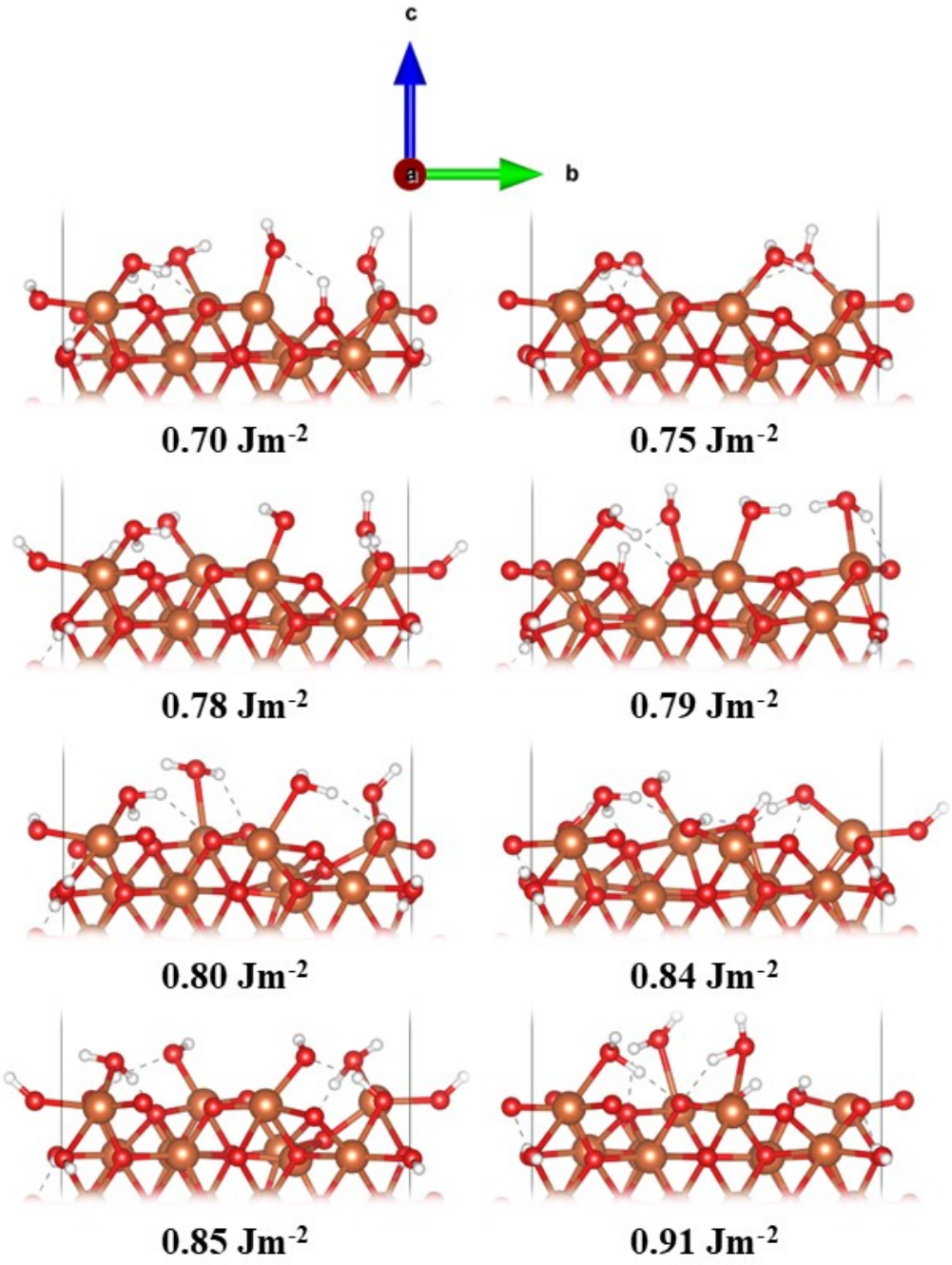

Figure S7: Hydrated Fh(110) surfaces and their corresponding γ_{hydr} surface energies. Colour scheme: Fe, orange; O, red; H, white.

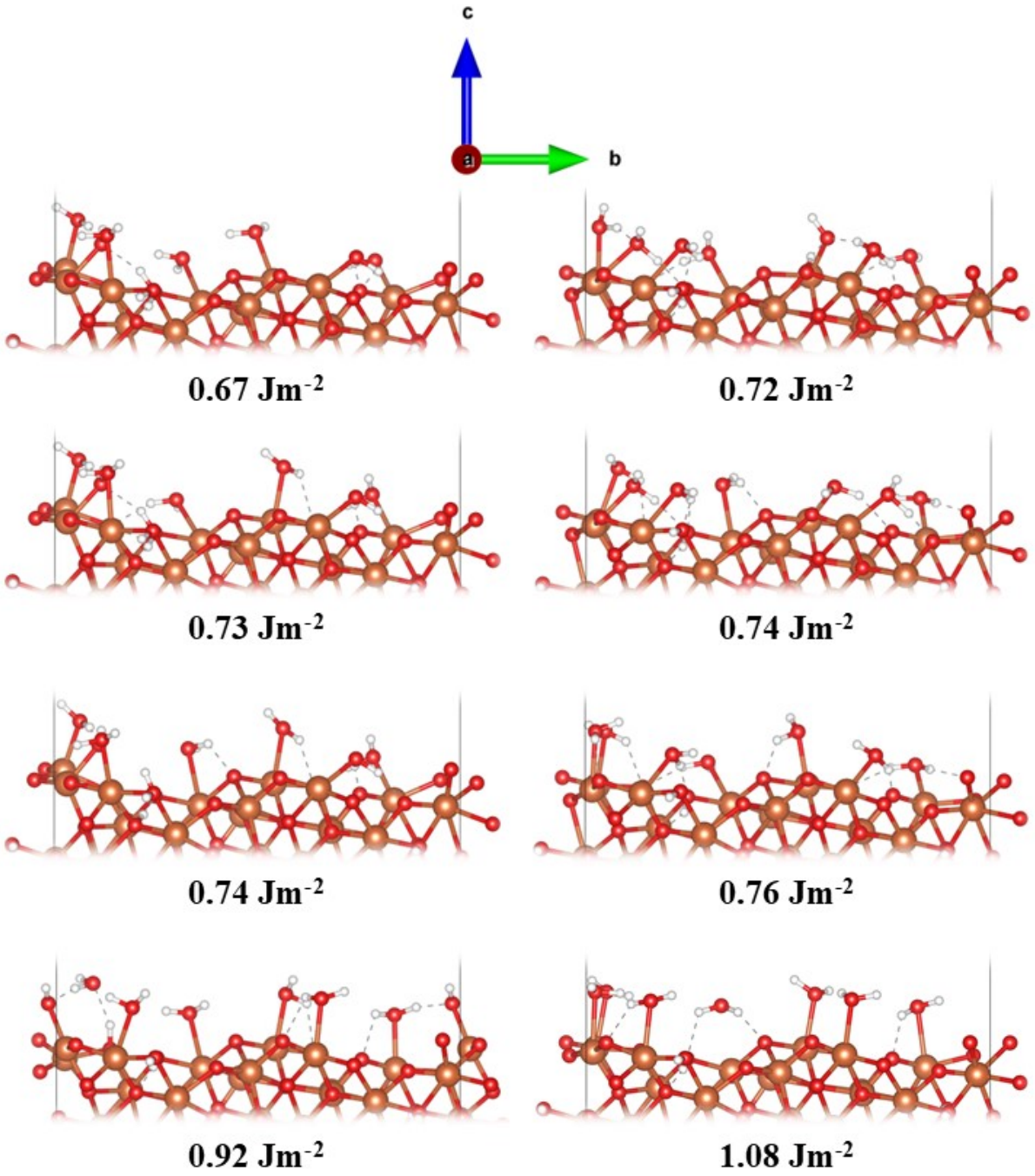

Figure S8: Hydrated Fh(120) surfaces and their corresponding γ_{hydr} surface energies. Colour scheme: Fe, orange; O, red; H, white.

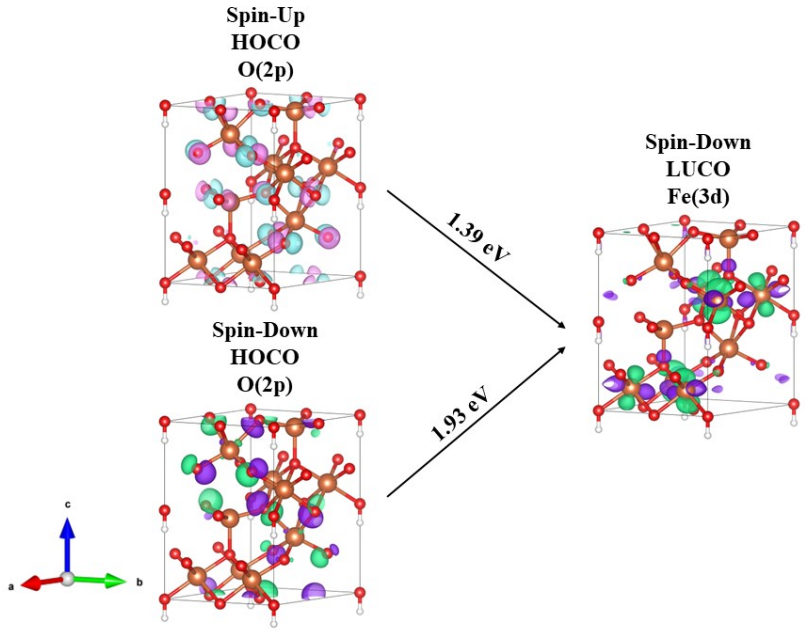

Figure S9: Real space wavefunctions (VASPKIT 511) for the valence band maximum at Γ and M and conduction band minimum at Γ showing O(2p) → Fe(3d) transitions. Spin-up orbitals are noted with pink and blue phases and spin-down orbitals are noted with purple and green phases.

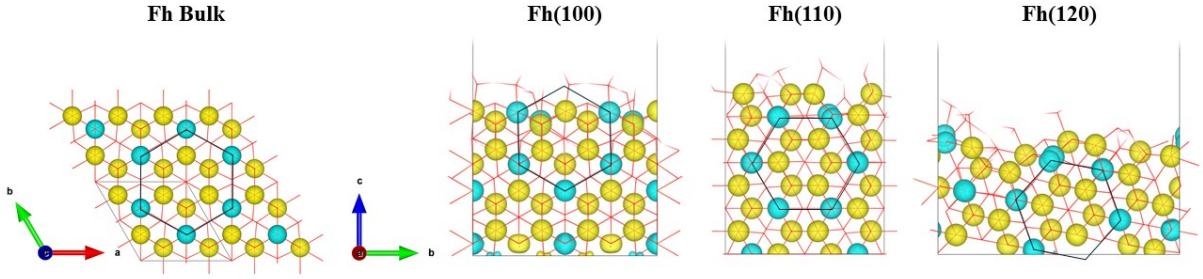

Figure S10: Comparison between the bulk spin density and lowest energy hydrated surfaces spin densities. Atoms and bonds are presented with the wireframe for clarity, and spin densities are presented with default VESTA settings. The black hexagon highlights that the relative position of spin-down Fe centres is preserved from bulk to relaxed, hydrated surface. Colour scheme: spin-up; yellow, spin-down; blue.

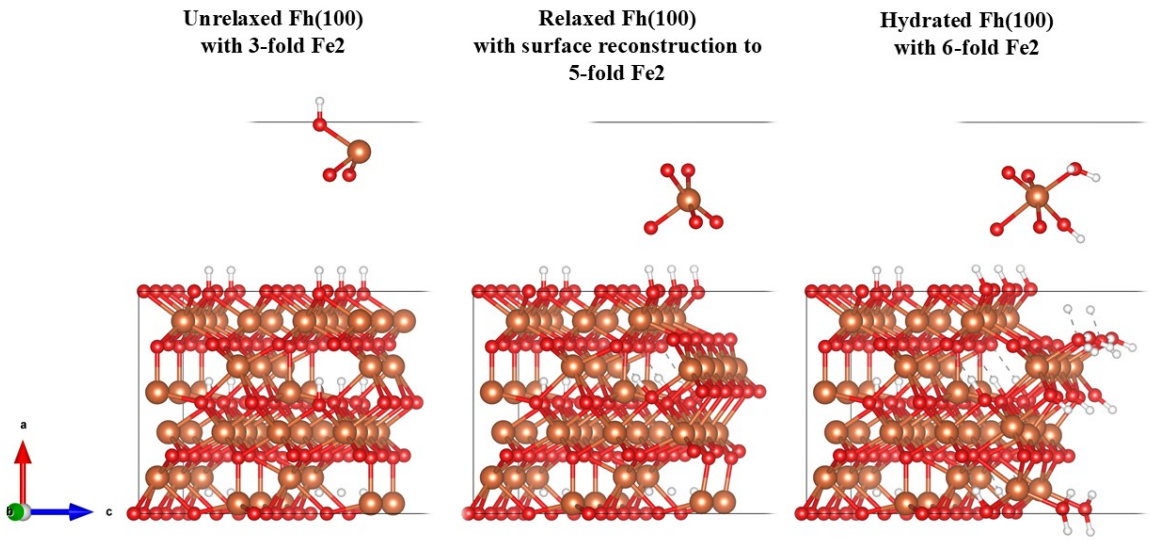

Figure S11: Fh(100) surface reconstruction showing how $Fe2_{Oh}$ shifts significantly during optimisation to regain a more stable coordination.

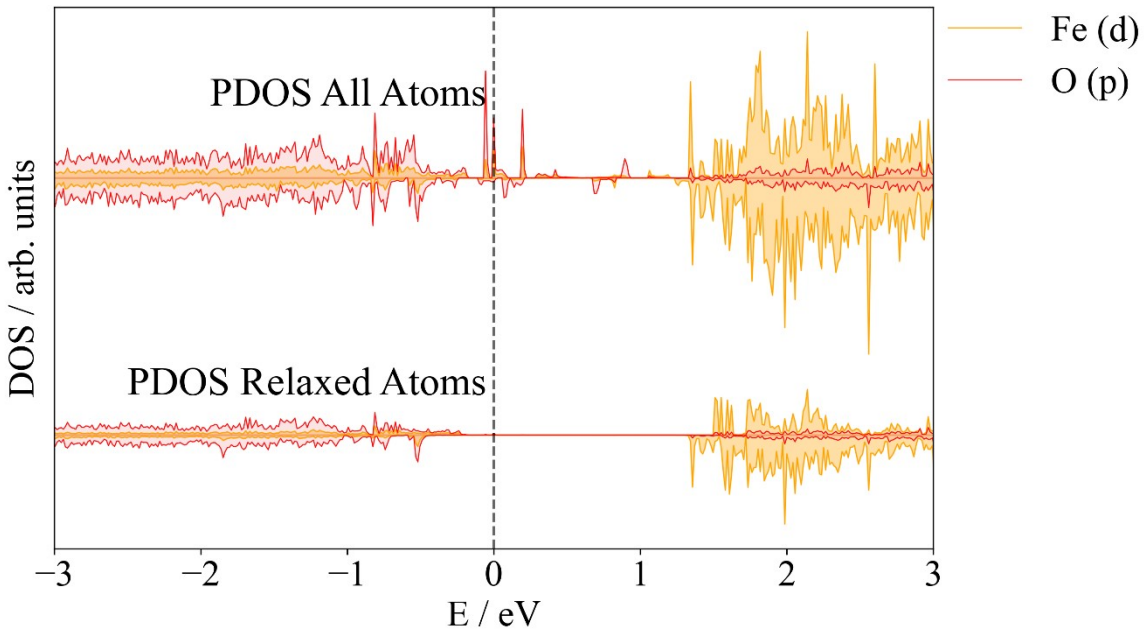

Figure S12: Fh(100) slab pDOS showing that defect states in the band gap are associated with fixed atoms. E = 0 eV represents the valence band maximum.

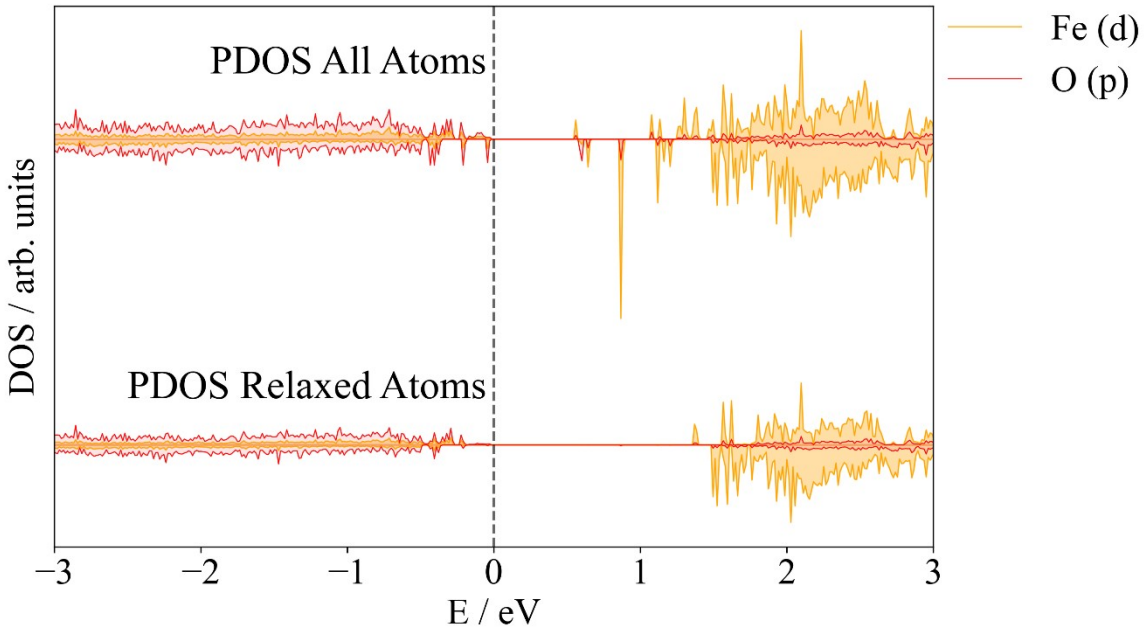

Figure S13: Fh(110) surface pDOS showing that defect states in the band gap are associated with fixed atoms. $E = 0$ eV represents the valence band maximum.

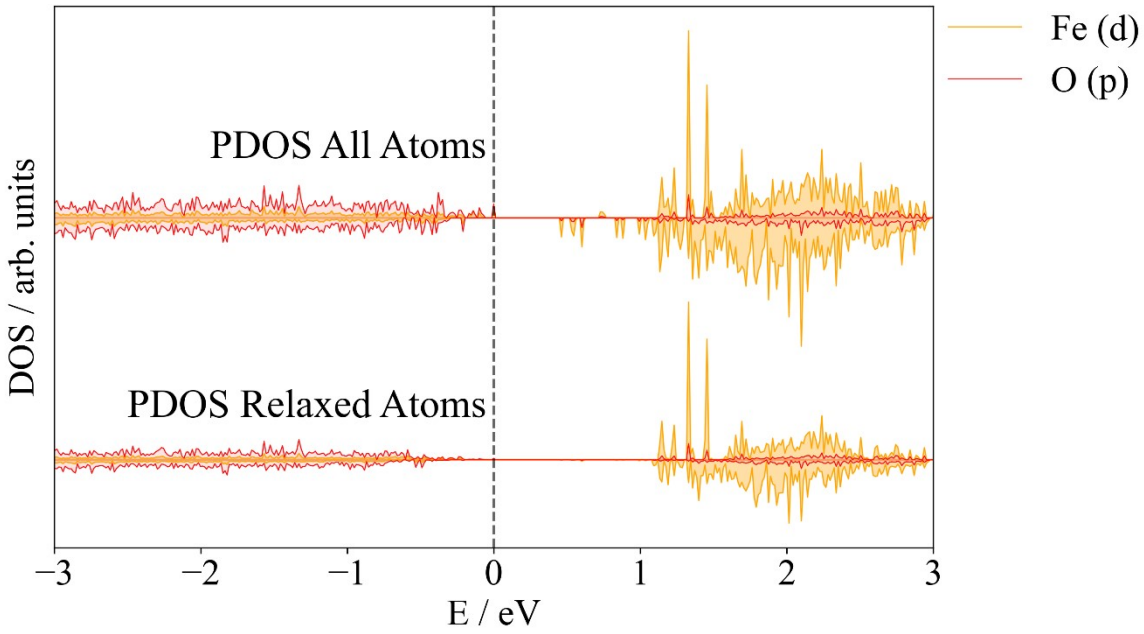

Figure S14: Fh(120) surface pDOS showing that defect states in the band gap are associated with fixed atoms. $E = 0$ eV represents the valence band maximum.

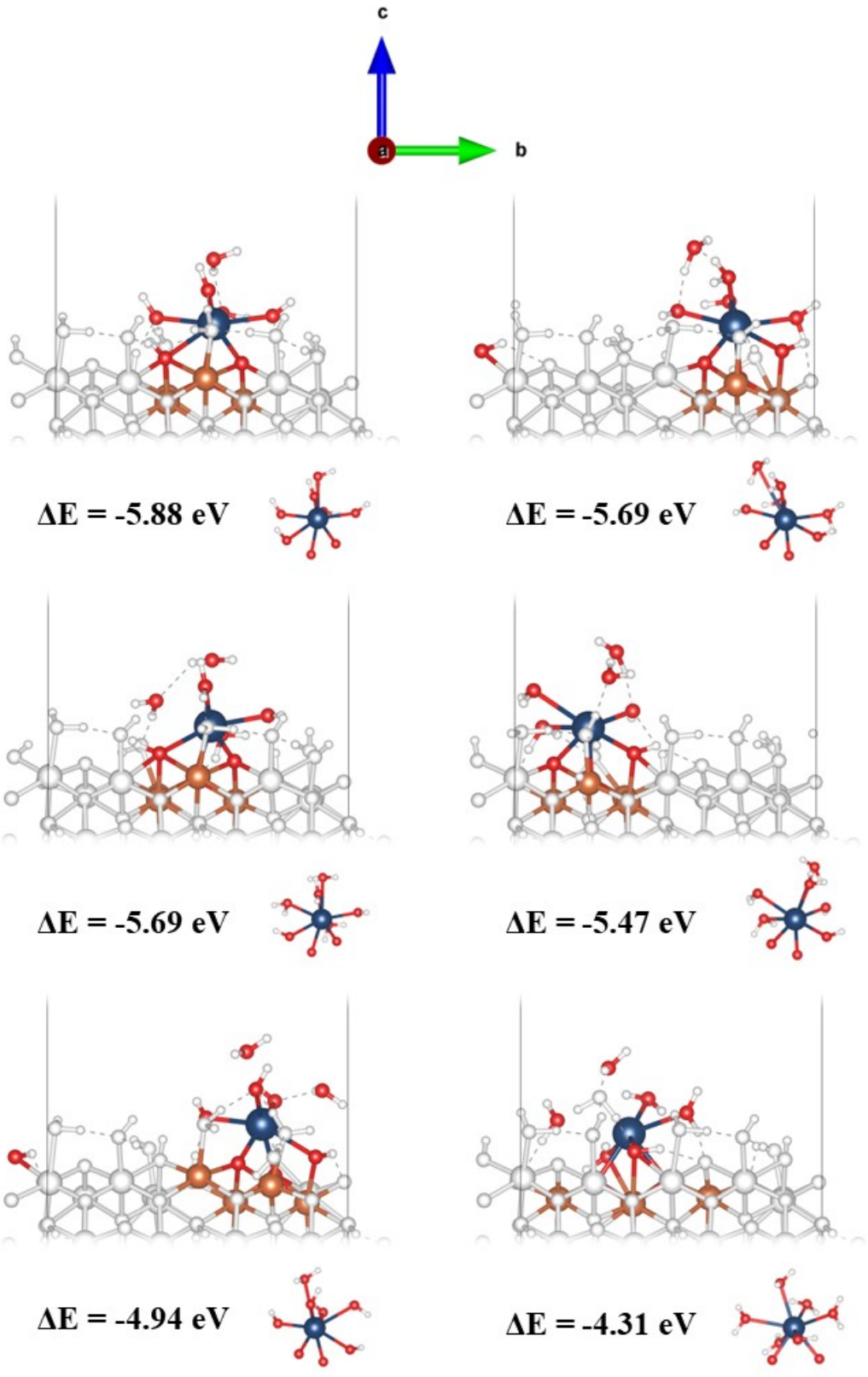

Figure S15: Pu@Fh(100) complexes and their corresponding reaction energies, Δ*E*. The closest eight O atoms and four Fe atoms are coloured and the Pu-O coordination is highlighted separately. Colour scheme: Fe, orange; O, red; H, white.

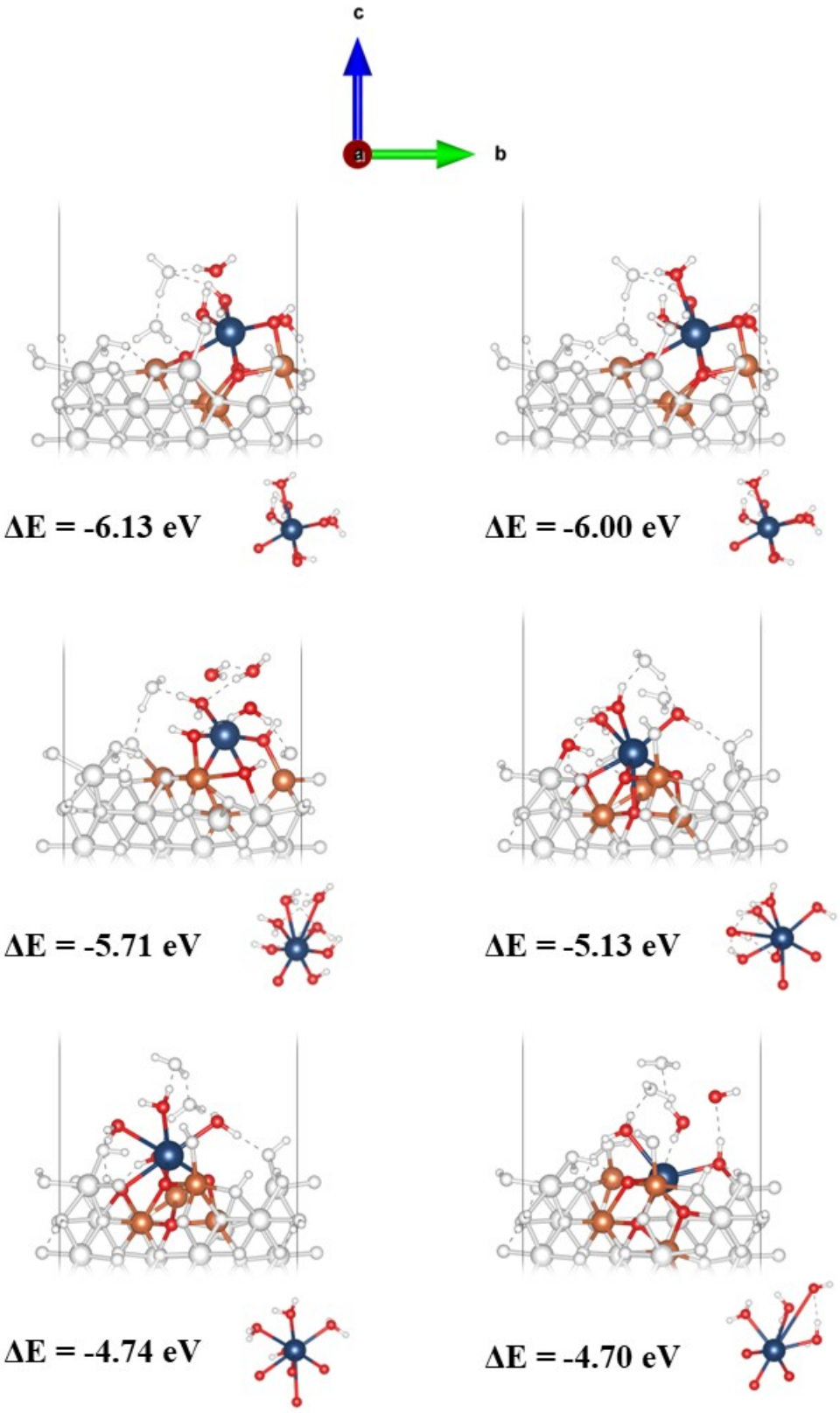

Figure S16: Pu@Fh(110) complexes and their corresponding reaction energies, Δ*E*. The closest eight O atoms and four Fe atoms are coloured and the Pu-O coordination is highlighted separately. Colour scheme: Fe, orange; O, red; H, white,

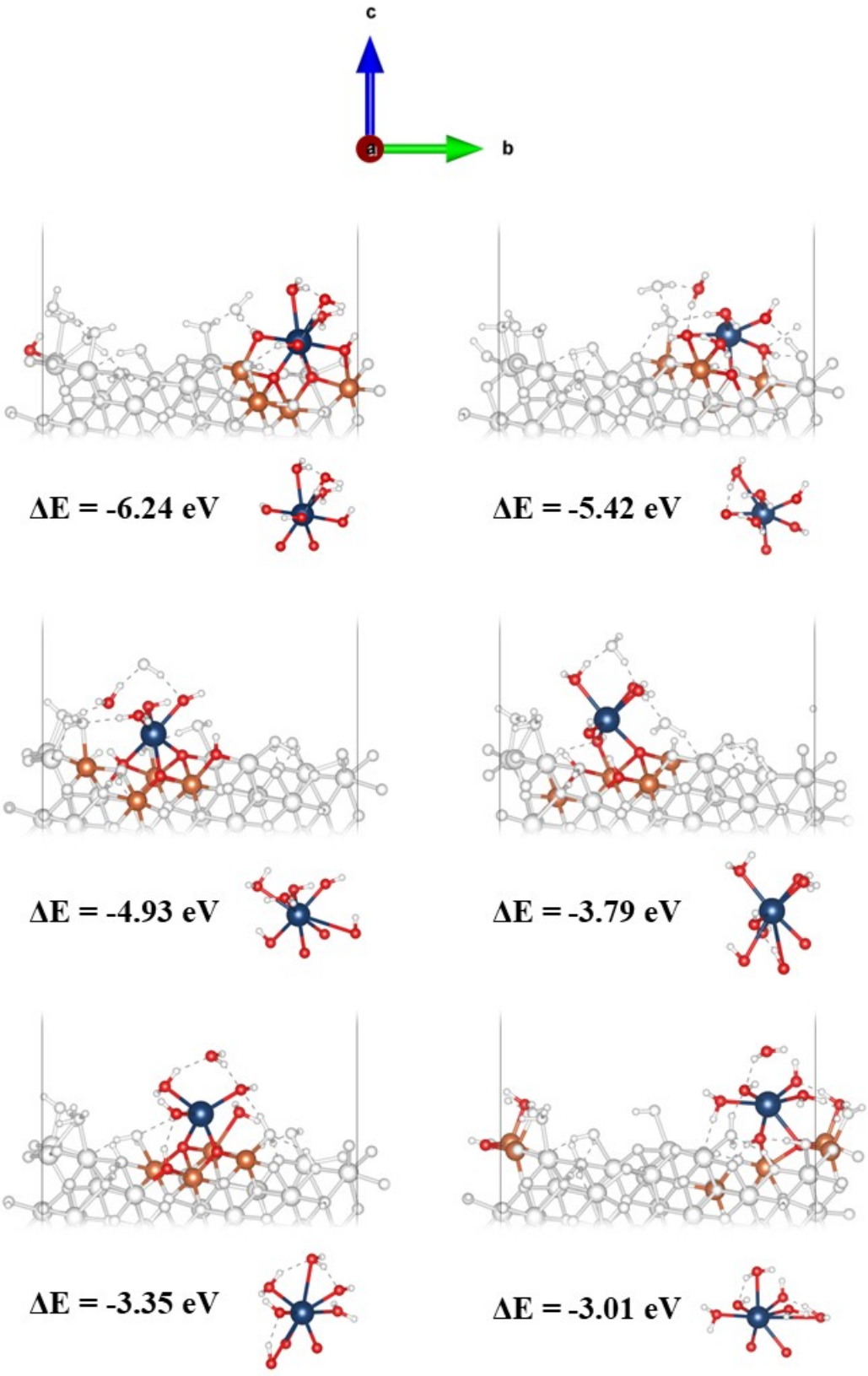

Figure S17: Pu@Fh(120) complexes and their corresponding reaction energies, Δ*E*. The closest eight O atoms and four Fe atoms are coloured and the Pu-O coordination is highlighted separately. Colour scheme: Fe, orange; O, red; H, white.

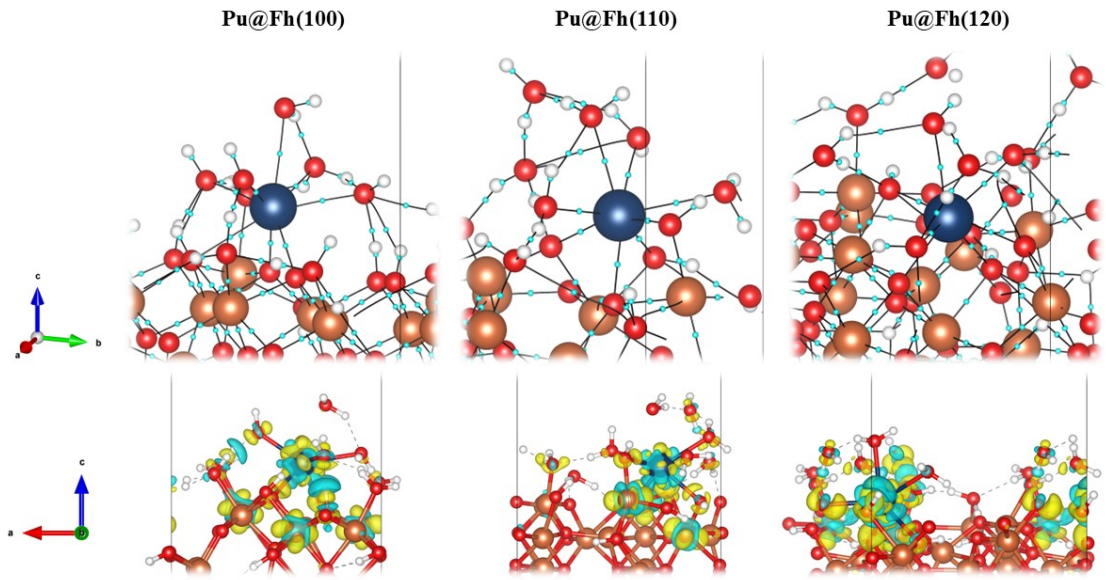

Figure S18: Analysis of the charge density surrounding the adsorbed Pu atom in the lowest energy Pu@Fh complexes. Upper; QTAIM molecular graph with BCPs coloured cyan. Lower; Charge density difference. Regions of charge accumulation and charge depletion are yellow and blue respectively. Surface presented with an isovalue = 0.01 eÅ^{-3}.

Supplementary Tables

Table S1: Fh bulk lattice parameters relaxed while varying U_{eff} and keeping a fixed 7×7×3 ***k***-point mesh and plane wave cutoff of 600 eV.

U_{eff} / eV	a = b / Å	c / Å	c/a	Spin-up Band Gap / eV	Spin-down Band Gap / eV	Direct Band Gap / eV
No U_{eff}	5.84	9.33	1.60	0.00	0.00	0.00
1	5.89	9.34	1.59	0.03	0.02	0.00
2	5.91	9.33	1.58	1.01	1.07	0.48
3	5.93	9.31	1.57	1.38	1.52	0.94
4	5.93	9.29	1.57	1.63	1.93	1.39
5	5.93	9.27	1.56	1.83	2.31	1.82

Table S2: Energy and lattice parameters for the relaxed Fh bulk while varying spin arrangement.

Spin Arrangement	SCF Energy / eV	a = b / Å	c / Å	c/a
Fe_1(Oh) ↑ Fe_2(Oh) ↓ Fe_3 (Td) ↓	-190.26341	5.93	9.29	1.57
Fe_1(Oh) ↑ Fe_2(Oh) ↓ Fe_3 (Td) ↑	-189.50240	5.96	9.29	1.56
Fe_1(Oh) ↑ Fe_2(Oh) ↑ Fe_3 (Td) ↓	-189.43593	5.96	9.25	1.55
Fe_1(Oh) ↑ Fe_2(Oh) ↑ Fe_3 (Td) ↑	-188.07947	5.99	9.27	1.55
no spin-polarisation	-169.00039	5.67	8.82	1.56

Table S3: Fh bulk convergence behaviour varying ***k***-points with a fixed plane wave energy cutoff of 600 eV and U_{eff} = 4 eV on Fe.

***k*-points**	**SCF Energy / eV**	**SCF Energy per atom / eV**
3×3×3	-189.632	-6.77259
5×5×3	-189.638	-6.77277
7×7×3	-189.638	-6.77278
9×9×3	-189.638	-6.77278
11×11×3	-189.638	-6.77278

Table S4: Fh bulk convergence behaviour varying plane wave energy cutoff with a fixed 7×7×3 ***k***-point mesh and U_{eff} = 4 eV on Fe.

ENCUT	SCF Energy / eV	SCF Energy per atom / eV
250	-194.422	-6.94364
300	-192.006	-6.85736
350	-190.488	-6.80315
400	-189.912	-6.78256
450	-189.662	-6.77364
500	-189.594	-6.77120
550	-189.604	-6.77156
600	-189.638	-6.77279
650	-189.667	-6.77384
700	-189.692	-6.77470

Table S5: Fh(100) convergence behaviour varying ***k***-points with a fixed plane wave energy cutoff of 600 eV.

***k*-points**	**SCF Energy / eV**	**SCF Energy per atom / eV**
1×1×1	-715.78770	-6.39096
3×3×1	-716.29426	-6.39548
5×5×1	-716.29736	-6.39551
7×7×1	-716.29745	-6.39551
9×9×1	-716.29757	-6.39551

Table S6: Fh(110) convergence behaviour varying ***k***-points with a fixed plane wave energy cutoff of 600 eV.

***k*-points**	**SCF Energy / eV**	**SCF Energy per atom / eV**
1×1×1	-736.18456	-6.57308
3×3×1	-736.33513	-6.57442
5×5×1	-736.33541	-6.57442
7×7×1	-736.33518	-6.57442
9×9×1	-736.33535	-6.57442

Table S7: Fh(120) convergence behaviour varying ***k***-points with a fixed plane wave energy cutoff of 600 eV.

***k*-points**	**SCF Energy / eV**	**SCF Energy per atom / eV**
1×1×1	-717.08611	-6.40255
3×3×1	-717.25271	-6.40404
5×5×1	-717.25293	-6.40404
7×7×1	-717.25305	-6.40405
9×9×1	-717.25295	-6.40404

Table S8: Fh(100) convergence behaviour of the surface energy with respect to layer relaxation.

#Layers Relaxed	SCF Energy / eV	SCF Energy per atom / eV	γ / Jm^{-2}
0	-716.29736	-6.39551	3.25
1	-719.03455	-6.41995	2.86
2	-720.14649	-6.42988	2.69
3	-721.38669	-6.44095	2.51
4	-726.22067	-6.48411	1.81
5	-726.49930	-6.48660	1.77
6	-726.90662	-6.49024	1.71
7	-726.96966	-6.49080	1.70

Table S9: Fh(110) convergence behaviour of the surface energy with respect to layer relaxation.

#Layers Relaxed	SCF Energy / eV	SCF Energy per atom / eV	γ / Jm^{-2}
0	-736.33541	-6.57442	2.07
1	-736.30653	-6.57417	2.08
2	-737.40129	-6.58394	1.90
3	-737.92978	-6.58866	1.81
4	-737.78637	-6.58738	1.83
5	-737.76894	-6.58722	1.83

Table S10: Fh(120) convergence behaviour of the surface energy with respect to layer relaxation.

#Layers Relaxed	SCF Energy / eV	SCF Energy per atom / eV	γ / Jm^{-2}
0	-717.25293	-6.40404	2.41
1	-718.14655	-6.41202	2.31
2	-722.20164	-6.44823	1.86
3	-723.75546	-6.46210	1.69
4	-724.49927	-6.46874	1.61
5	-724.72568	-6.47077	1.59
6	-724.80773	-6.47150	1.58

Table S11: Fh surface hydration energies corresponding with figures S6–S8.

Surface ID	SCF Energy / eV	γ_{hydr} / Jm^{-2}	Average Fe-O$_{surf}$ / Å	Did water dissociate?*
Fh(100)				
1	-820.55835	0.50	2.07	yes
2	-819.67280	0.63	2.27	no
3	-819.52486	0.65	2.09	yes
4	-819.40517	0.67	2.24	no
5	-819.31794	0.68	2.19	yes
6	-819.18054	0.70	2.33	yes[a]
7	-819.09994	0.71	2.27	no
8	-818.60216	0.79	2.35	no[a]
Fh(110)				
1	-801.43656	0.70	1.99	yes
2	-801.14079	0.75	2.05	yes
3	-800.95721	0.78	1.97	yes
4	-800.79928	0.80	2.09	yes
5	-800.55711	0.84	2.01	yes
6	-800.54646	0.85	1.98	yes
7	-800.30415	0.89	2.10	yes
8	-800.16296	0.91	2.17	yes
Fh(120)				
1	-832.60187	0.67	2.14	yes
2	-832.16042	0.72	2.17	yes
3	-832.03506	0.73	2.15	yes
4	-831.99034	0.74	2.19	no
5	-831.95607	0.74	2.15	yes
6	-831.77687	0.76	2.17	no
7	-830.34035	0.92	2.35	yes[a]
8	-828.90712	1.08	2.31	no[a]

* Dissociation refers to the process where $H_2O \rightarrow OH^- + H^+$, in the cases marked with [a] we see H_2O desorb from the surface hence the larger average distance and higher γ_{hydr}.

Table S12: Pu@Fh reaction energies, charge, and average Pu-O/Fe corresponding with figures S15–S17.

Surface ID	ΔE_r / eV	q(Pu)	Average distance to n closest Pu-O / Å			Average distance to 4 closest Pu-Fe / Å	Binding Mode
			n = 6	n = 7	n = 8		
Fh(100)							
1	-5.88	2.13	2.47	2.50	2.53	3.65	tridentate
2	-5.69	2.12	2.45	2.48	2.61	3.56	tridentate
3	-5.69	2.11	2.48	2.51	2.54	3.61	tridentate
4	-5.47	2.12	2.45	2.49	2.59	3.51	tridentate
5	-4.94	2.11	2.46	2.51	2.57	3.63	tridentate
6	-4.31	2.12	2.49	2.52	2.57	3.57	tridentate
Fh(110)							
1	-6.13	2.13	2.48	2.51	2.54	3.55	tetradentate
2	-6.02	2.11	2.47	2.53	2.63	3.61	tetradentate
3	-5.71	2.04	2.48	2.56	2.66	3.33	tetradentate
4	-5.15	2.05	2.49	2.51	2.63	3.26	tetradentate
5	-4.74	2.04	2.47	2.56	2.76	3.26	tridentate
6	-4.70	2.03	2.48	2.51	2.53	3.52	tetradentate
Fh(120)							
1	-6.24	2.15	2.45	2.47	2.58	3.61	tetradentate
2	-5.42	2.14	2.43	2.48	2.62	3.72	tetradentate
3	-4.93	2.12	2.47	2.50	2.62	3.71	tridentate
4	-3.79	2.15	2.45	2.50	2.66	4.02	bidentate
5	-3.35	2.10	2.47	2.57	2.69	3.73	bidentate
6	-3.01	2.07	2.47	2.50	2.67	4.09	bidentate

Table S13: Average Pu-O QTAIM bond critical point properties (a.u.) for the Pu@Fh complexes.

Surface ID	Pu-O_{surf}			Pu-O_{water}			Overall Pu-O		
	ρ	***H***	**-G/V**	***ρ***	***H***	**-G/V**	***ρ***	***H***	**-G/V**
Fh(100)									
1	0.07	-0.02	0.82	0.04	0.00	0.95	0.05	-0.01	0.90
2	0.07	-0.02	0.83	0.05	0.00	0.93	0.06	-0.01	0.89
3	0.07	-0.02	0.85	0.04	0.00	0.97	0.06	-0.01	0.89
4	0.07	-0.02	0.83	0.05	-0.01	0.94	0.06	-0.01	0.89
5	0.08	-0.02	0.81	0.05	0.00	0.93	0.05	-0.01	0.95
6	0.06	-0.01	0.86	0.03	0.00	1.02	0.05	-0.01	0.91
Fh(110)									
1	0.07	-0.02	0.84	0.02	0.00	0.99	0.05	-0.01	0.93
2	0.06	-0.01	0.85	0.04	0.00	0.99	0.05	-0.01	0.92
3	0.07	-0.02	0.84	0.02	0.00	1.14	0.05	-0.01	0.99
4	0.06	-0.01	0.86	0.04	0.00	0.92	0.05	-0.01	0.89
5	0.08	-0.02	0.82	0.04	0.00	0.96	0.06	-0.01	0.89
6	0.07	-0.02	0.82	0.03	0.00	1.06	0.05	-0.01	0.92
Fh(120)									
1	0.07	-0.02	0.85	0.04	0.00	0.93	0.06	-0.01	0.88
2	0.07	-0.01	0.84	0.05	0.00	0.96	0.06	-0.01	0.91
3	0.07	-0.01	0.86	0.05	-0.01	0.95	0.06	-0.01	0.91
4	0.06	-0.01	0.88	0.06	-0.01	0.89	0.05	-0.01	0.91
5	0.09	-0.03	0.78	0.05	-0.01	0.97	0.06	-0.01	0.91
6	0.05	-0.01	0.90	0.05	-0.01	0.90	0.05	-0.01	0.90

Optimised Coordinates

All coordinates given in the VASP POSCAR format.

Bulk Fh – Fe10O16H2

1.0

5.9329633713	0.0000000000	0.0000000000
-2.9664816856	5.1380969992	0.0000000000
0.0000000000	0.0000000000	9.2860965729

Fe O H

10 16 2

Direct

0.332600892	0.166300446	0.124017119
0.833699524	0.667399108	0.124017119
0.833699524	0.166300446	0.124017119
0.667399108	0.833699524	0.624017119
0.166300446	0.332600892	0.624017119
0.166300446	0.833699524	0.624017119
0.333333343	0.666666687	0.327588290
0.666666627	0.333333313	0.827588260
0.666666687	0.333333343	0.444383085
0.333333313	0.666666627	0.944383025
0.000000000	0.000000000	0.001627103
0.000000000	0.000000000	0.501627088
0.514325798	0.028651608	0.990150630
0.514325738	0.485674173	0.990150630
0.971348405	0.485674232	0.990150630
0.485674173	0.971348405	0.490150660
0.485674232	0.514325798	0.490150660
0.028651608	0.514325738	0.490150660
0.166437313	0.332874626	0.228600621
0.166437313	0.833562672	0.228600621
0.667125344	0.833562672	0.228600621
0.833562672	0.667125344	0.728600621
0.833562672	0.166437313	0.728600621
0.332874626	0.166437313	0.728600621
0.666666687	0.333333343	0.239424303
0.333333313	0.666666627	0.739424288
0.000000000	0.000000000	0.895672083
0.000000000	0.000000000	0.395672113

Relaxed Fh(100) – Fe40O64H8

1.0

9.2869243622	0.0000000000	0.0000000000
0.0000000000	11.8661737442	0.0000000000
0.0000000000	0.0000000000	30.1291179657

Fe O H

40 64 8

Direct

0.162497729	0.000000000	0.025979901
0.162497729	0.500000000	0.025979901
0.545726061	0.000000000	0.025979908
0.545726061	0.500000000	0.025979908
0.366069466	0.250000030	0.026101509
0.366069466	0.750000000	0.026101509
0.866069496	0.125267372	0.054463953
0.866069496	0.625267386	0.054463953
0.866069496	0.374732584	0.054463953
0.866069496	0.874732614	0.054463953
0.366069466	0.374732584	0.111188836
0.366069466	0.874732614	0.111188836
0.366069466	0.125267401	0.111188836
0.366069466	0.625267386	0.111188836
0.866069496	0.250000000	0.139551282
0.866069496	0.750000000	0.139551282
0.045726035	0.000000000	0.139672890
0.045726035	0.500000000	0.139672890
0.662497759	0.000000000	0.139672890
0.662497759	0.500000000	0.139672890
0.166670874	0.250000000	0.196850047
0.166670874	0.750000000	0.196850047
0.548743725	0.250000000	0.195786014
0.548743725	0.750000000	0.195786014
0.364092618	0.000000000	0.198437989
0.364092618	0.500000000	0.198437989
0.875141799	0.377696842	0.226518705
0.875141799	0.877696872	0.226518705
0.875141799	0.122303128	0.226518705
0.875141799	0.622303128	0.226518705
0.359576195	0.129364282	0.286711723
0.359576195	0.629364312	0.286711723
0.359576195	0.370635718	0.286711723
0.359576195	0.870635688	0.286711723
0.648714125	0.000000000	0.304909706
0.648714125	0.500000000	0.304909706
0.051913567	0.249999985	0.304545790
0.051913567	0.750000000	0.304545790
0.656866074	0.250000000	0.307171911
0.656866074	0.750000000	0.307171911
0.999996483	0.114250407	0.000000963
0.999996483	0.614250422	0.000000963
0.999996483	0.385749578	0.000000970
0.999996483	0.885749519	0.000000970
0.750683308	0.000000000	0.025979908
0.750683308	0.500000000	0.025979908
0.761544108	0.250000000	0.026044222
0.761544108	0.750000000	0.026044222
0.261544079	0.374858558	0.054435298
0.261544079	0.874858558	0.054435298
0.261544079	0.125141427	0.054435298
0.261544079	0.625141442	0.054435298
0.999996483	0.000000000	0.077937789
0.999996483	0.500000000	0.077937789
0.988357246	0.250000000	0.082826398
0.988357246	0.750000000	0.082826398
0.488357216	0.250000000	0.082826398
0.488357216	0.750000000	0.082826398
0.499996394	0.000000000	0.087715007
0.499996394	0.500000000	0.087715007
0.761544108	0.374858558	0.111217491
0.761544108	0.874858558	0.111217491
0.761544108	0.125141427	0.111217491
0.761544108	0.625141442	0.111217491
0.261544079	0.250000000	0.139608577
0.261544079	0.750000000	0.139608577
0.250683278	0.000000000	0.139672890
0.250683278	0.500000000	0.139672890
0.499996394	0.114250422	0.165651828
0.499996394	0.614250422	0.165651828
0.499996394	0.385749578	0.165651858
0.499996394	0.885749519	0.165651858
0.999996483	0.364250392	0.170540452
0.999996483	0.864250422	0.170540452
0.999996483	0.135749578	0.170540452
0.999996483	0.635749578	0.170540452
0.753320038	0.250000000	0.198167101
0.753320038	0.750000000	0.198167101
0.752522588	0.000000000	0.200665876
0.752522588	0.500000000	0.200665876
0.264190018	0.124755137	0.225821584

0.264190018	0.624755144	0.225821584
0.264190018	0.375244856	0.225821584
0.264190018	0.875244796	0.225821584
0.001698960	0.250000030	0.244085208
0.001698960	0.750000000	0.244085208
0.995109379	0.000000000	0.252220362
0.995109379	0.500000000	0.252220362
0.523504019	0.000000000	0.250423402
0.523504019	0.500000000	0.250423402
0.495475411	0.250000000	0.256476074
0.495475411	0.750000000	0.256476074
0.782765210	0.132174537	0.289184272
0.782765210	0.632174551	0.289184272
0.782765210	0.367825449	0.289184272
0.782765210	0.867825389	0.289184272
0.280341774	0.000000000	0.309696913
0.280341774	0.500000000	0.309696913
0.248884872	0.249999985	0.314597219
0.248884872	0.750000000	0.314597219
0.549204588	0.368998379	0.330055565
0.549204588	0.868998408	0.330055565
0.549204588	0.131001651	0.330055594
0.549204588	0.631001592	0.330055594
0.094305724	0.250000000	0.082826398
0.094305724	0.750000000	0.082826398
0.594305754	0.250000000	0.082826398
0.594305754	0.750000000	0.082826398
0.099418804	0.000000000	0.246743053
0.099418804	0.500000000	0.246743053
0.608938932	0.000000000	0.228331491
0.608938932	0.500000000	0.228331491

Relaxed Fh(110) – Fe40O64H8

1.0

9.2869243622	0.0000000000	0.0000000000
0.0000000000	10.2764081955	0.0000000000
0.0000000000	0.0000000000	31.8661727905

Fe	O	H
40	64	8

Direct

0.674137771	0.833333373	0.000000000
0.057366032	0.833333313	0.000000000
0.557366073	0.166666687	0.000000000
0.174137741	0.166666687	0.000000000
0.877709508	0.333689868	0.000000000
0.377709448	0.666310132	0.000000000
0.877709508	0.583155096	0.046443813
0.377709448	0.416844964	0.046443813
0.377709448	0.916844845	0.046642952
0.877709508	0.083155155	0.046642952
0.674137771	0.333333373	0.093090288
0.557366073	0.666666627	0.093090288
0.057366032	0.333333313	0.093090288
0.174137741	0.666666687	0.093090288
0.877709508	0.833689809	0.093090288
0.377709448	0.166310191	0.093090288
0.877709508	0.083155155	0.139537632
0.377709448	0.916844964	0.139537632
0.377709448	0.416844904	0.139736772
0.877709508	0.583155155	0.139736772
0.677259505	0.832683980	0.186498791
0.559548676	0.173894823	0.186912149
0.058611397	0.831742823	0.186848924
0.172915772	0.164567456	0.186966643
0.875517428	0.335301608	0.188028932
0.371120542	0.664835513	0.188063517
0.873288393	0.587874532	0.232700393
0.375775009	0.409406066	0.232679173
0.394566596	0.929936826	0.230024725
0.873906612	0.076110341	0.231388927
0.672323048	0.340216786	0.284747362
0.542764008	0.672504067	0.277573675
0.060623016	0.322337985	0.279697508
0.186894178	0.629607797	0.292840302
0.896650493	0.830866337	0.284031272
0.385960102	0.160448432	0.286421537
0.894999623	0.097468123	0.319524050
0.357574522	0.909695745	0.323126674
0.385682255	0.411929339	0.323756933
0.882312179	0.570686698	0.321229517
0.511636436	0.757166386	0.957452476
0.762323320	0.166666687	0.000000000
0.511636436	0.985667229	0.000000000
0.499997169	0.500000000	0.000000000
0.999997258	0.500000000	0.000000000
0.773184121	0.666478097	0.000000000
0.273184061	0.333521903	0.000000000
0.262323260	0.833333313	0.000000000
0.011636457	0.014332831	0.000000000
0.011636457	0.242833614	0.042540543
0.511636436	0.757166386	0.042540543
0.273184061	0.583239079	0.046490721
0.773184121	0.416760981	0.046490721
0.773184121	0.916760862	0.046596043
0.273184061	0.083239138	0.046596043
0.011636457	0.742833614	0.050546281
0.511636436	0.257166386	0.050546281
0.762323320	0.666666627	0.093090288
0.511636436	0.485667229	0.093090288
0.499997169	0.000000000	0.093090288
0.999997258	0.000000000	0.093090288
0.773184121	0.166478157	0.093090288
0.273184061	0.833521843	0.093090288
0.262323260	0.333333313	0.093090288
0.011636457	0.514332771	0.093090288
0.011636457	0.742833614	0.135634303
0.511636436	0.257166386	0.135634303
0.273184061	0.083239138	0.139584541
0.773184121	0.916760862	0.139584541
0.773184121	0.416760981	0.139689863
0.273184061	0.583239079	0.139689863
0.011636457	0.242833555	0.143640101
0.511636436	0.757166386	0.143640101
0.762945235	0.167148024	0.186066866
0.515127599	0.991823792	0.185119852
0.496337414	0.499654800	0.186975926
0.997121572	0.501685858	0.186951771
0.769465029	0.665258288	0.185974881
0.272249937	0.330405414	0.185984656
0.264942765	0.835917950	0.188234225
0.010758224	0.012959513	0.185584918
0.010041886	0.239441574	0.227901950
0.509705365	0.761906981	0.226450026
0.271617055	0.580041468	0.235842437
0.768769145	0.420057178	0.233678684
0.771287680	0.915517271	0.234503999
0.268827289	0.075191423	0.235171735
0.004162400	0.745916605	0.235678300
0.511725068	0.256643385	0.237116307
0.752882957	0.676581919	0.283138394
0.506982446	0.492719173	0.280034214
0.507004917	0.990254581	0.280000329
0.014802681	0.003628454	0.276097953
0.773142755	0.168435454	0.279439628

0.372406900	0.738519847	0.304581136
0.264676809	0.324067950	0.279236108
0.010002915	0.502011359	0.277441949
0.017722750	0.716822922	0.319937438
0.512491226	0.270543307	0.321809828
0.281080961	0.072681040	0.327521145
0.813318312	0.943306386	0.327973813
0.765833139	0.434722275	0.327600747
0.244566336	0.521897614	0.336895555
0.004748333	0.234490529	0.327528149
0.605945766	0.500000000	0.000000000
0.105945729	0.500000000	0.000000000
0.605945766	0.000000000	0.093090288
0.105945729	0.000000000	0.093090288
0.602502465	0.500652194	0.187845871
0.102787405	0.502439797	0.189056695
0.612890482	0.989501715	0.278631955
0.116826706	0.027720964	0.269115627

Relaxed Fh(120) – Fe40O64H8

1.0

9.2869243622	0.0000000000	0.0000000000
0.0000000000	15.6974725723	0.0000000000
0.0000000000	0.0000000000	27.7125644684

Fe	O	H
40	64	8

Direct

0.866069436	0.895775735	0.010574830
0.045726012	0.395928562	0.010674772
0.662497699	0.395928562	0.010674779
0.366069436	0.788862050	0.022229623
0.366069436	0.288556516	0.022379527
0.866069436	0.074729197	0.045689102
0.866069436	0.574423611	0.045839008
0.162497714	0.967357099	0.057393853
0.545726001	0.967357099	0.057393868
0.366069436	0.467509985	0.057493795
0.866069436	0.252918661	0.080653481
0.045726012	0.753071368	0.080753393
0.662497699	0.753071368	0.080753408
0.366069436	0.146004975	0.092308275
0.366069436	0.645699441	0.092458174
0.866069436	0.431872129	0.115767762
0.866069436	0.931566477	0.115917645
0.162497714	0.324500024	0.127472505
0.545726001	0.324500024	0.127472505
0.366069436	0.824652791	0.127572432
0.866064906	0.611325920	0.149973810
0.046715286	0.111992352	0.147734061
0.656777501	0.114614904	0.150928259
0.363939226	0.504274666	0.161001399
0.379187047	0.004631115	0.157219857
0.878187478	0.790915787	0.188075781
0.874814808	0.296515852	0.192557603
0.160860255	0.682021558	0.202464342
0.550649703	0.684633493	0.198341280
0.350711524	0.179665834	0.206475168
0.876659095	0.968614936	0.224583879
0.023534179	0.456676573	0.219811052
0.674954236	0.479239792	0.228830427
0.386300176	0.841777146	0.233691514
0.390621632	0.360993922	0.230310559
0.849767089	0.140249088	0.247082010
0.874817610	0.641256213	0.251706928
0.174148753	0.023594899	0.258000344
0.546089292	0.016138973	0.258051902
0.365464151	0.540880084	0.260459870
0.499996364	0.493857563	0.999999404
0.999996424	0.000000000	0.004017139
0.261544049	0.895847678	0.010621910
0.250683248	0.395928562	0.010674772
0.761544049	0.788826108	0.022288477
0.761544049	0.288664460	0.022367772
0.999996424	0.675500274	0.030016633
0.988357186	0.181642890	0.034034315
0.488357157	0.181642890	0.034034315
0.499996364	0.687785506	0.038052000
0.261544049	0.074621253	0.045700874
0.261544049	0.574459612	0.045780148
0.750683248	0.967357099	0.057393868
0.761544049	0.467437983	0.057446722
0.499996364	0.363285601	0.064051531
0.999996424	0.869428217	0.068069212
0.499996364	0.851000369	0.070078067
0.999996424	0.357143044	0.074095748
0.261544049	0.252990603	0.080700554
0.250683248	0.753071368	0.080753393
0.761544049	0.145968974	0.092367090
0.761544049	0.645807385	0.092446409
0.999996424	0.032643072	0.100095280
0.988357186	0.538785756	0.104112953
0.488357157	0.538785756	0.104112953
0.499996364	0.044928364	0.108130634
0.261544049	0.431764066	0.115779512
0.261544049	0.931602418	0.115858801
0.750683248	0.324500024	0.127472505
0.761544049	0.824580848	0.127525330
0.499996364	0.720428467	0.134130150
0.996625602	0.227772951	0.140807748
0.497159362	0.209373102	0.139029324
0.002680983	0.713313282	0.144438282
0.260158896	0.609359264	0.150656119
0.249407053	0.105739601	0.152600273
0.759767294	0.505159199	0.161622420
0.767477214	0.006529992	0.164296925
0.009174731	0.388023823	0.164403871
0.997195661	0.897321880	0.170929819
0.489391387	0.895484209	0.174764022
0.501722515	0.402703375	0.176292479
0.259760827	0.790583014	0.188415900
0.259799033	0.289010227	0.188213274
0.754790783	0.684134781	0.196817800
0.740661919	0.196360752	0.199342743
0.493079007	0.079726703	0.200741142
0.996624351	0.572935700	0.208599523
0.497806042	0.568402767	0.207330748
0.991188049	0.073604733	0.211400285
0.352397978	0.954473436	0.258036166
0.234591931	0.457829416	0.226850256
0.778310299	0.872982085	0.229976892
0.835890412	0.395041525	0.234100387
0.996589839	0.734244585	0.239851922
0.973188102	0.238547340	0.252565295
0.483020484	0.252088666	0.247116104
0.509007335	0.757947683	0.247642726
0.236596376	0.132975593	0.256204069
0.255222708	0.633893728	0.256714940
0.741530418	0.048323505	0.268139124
0.753605008	0.559510648	0.271061510
0.494017750	0.444875181	0.269836694
0.019995064	0.954498112	0.270097971
0.094305709	0.181642890	0.034034315
0.594305694	0.181642890	0.034034315
0.094305709	0.538785756	0.104112953

0.594305694 0.538785756 0.104112953
0.100611433 0.893677533 0.163104847
0.595677793 0.892183959 0.171431705
0.074519835 0.218778789 0.251255035
0.581945956 0.242480278 0.234888330

Hydrated Fh(100) – Fe40O64H8 • 6H2O

1.0

9.2869243622 0.0000000000 0.0000000000
0.0000000000 11.8661737442 0.0000000000
0.0000000000 0.0000000000 30.1291179657

Fe O H
40 70 20

Direct

0.162497729 0.000000000 0.025979901
0.162497729 0.500000000 0.025979901
0.545726061 0.000000000 0.025979908
0.545726061 0.500000000 0.025979908
0.366069466 0.250000030 0.026101509
0.366069466 0.750000000 0.026101509
0.866069496 0.125267372 0.054463953
0.866069496 0.625267386 0.054463953
0.866069496 0.374732584 0.054463953
0.866069496 0.874732614 0.054463953
0.366069466 0.374732584 0.111188836
0.366069466 0.874732614 0.111188836
0.366069466 0.125267401 0.111188836
0.366069466 0.625267386 0.111188836
0.866069496 0.250000000 0.139551282
0.866069496 0.750000000 0.139551282
0.045726035 0.000000000 0.139672890
0.045726035 0.500000000 0.139672890
0.662497759 0.000000000 0.139672890
0.662497759 0.500000000 0.139672890
0.162497729 0.250000000 0.196519375
0.162497729 0.750000000 0.196519375
0.545726061 0.250000000 0.196519375
0.545726061 0.750000000 0.196519375
0.366069466 0.000000000 0.196640968
0.366069466 0.500000000 0.196640968
0.863312602 0.377308697 0.225593030
0.863355219 0.877296686 0.225596115
0.876835227 0.125576794 0.227885053
0.876811802 0.625285804 0.227722645
0.351841718 0.123256065 0.287245929
0.351574302 0.623332441 0.287464947
0.389522910 0.367631912 0.280358255
0.390777647 0.867659330 0.280566335
0.661827981 0.004113782 0.310072154
0.661403239 0.503922939 0.309912801
0.108626164 0.367666841 0.288583905
0.110129274 0.868529081 0.287842125
0.660013020 0.241056725 0.307452053
0.661320806 0.741062701 0.307479262
0.999996483 0.114250407 0.000000963
0.999996483 0.614250422 0.000000963
0.999996483 0.385749578 0.000000970
0.999996483 0.885749519 0.000000970
0.750683308 0.000000000 0.025979908
0.750683308 0.500000000 0.025979908
0.761544108 0.250000000 0.026044222
0.761544108 0.750000000 0.026044222
0.261544079 0.374858558 0.054435298
0.261544079 0.874858558 0.054435298
0.261544079 0.125141427 0.054435298
0.261544079 0.625141442 0.054435298
0.999996483 0.000000000 0.077937789
0.999996483 0.500000000 0.077937789
0.988357246 0.250000000 0.082826398
0.988357246 0.750000000 0.082826398
0.488357216 0.250000000 0.082826398
0.488357216 0.750000000 0.082826398
0.499996394 0.000000000 0.087715007
0.499996394 0.500000000 0.087715007
0.761544108 0.374858558 0.111217491
0.761544108 0.874858558 0.111217491
0.761544108 0.125141427 0.111217491
0.761544108 0.625141442 0.111217491
0.261544079 0.250000000 0.139608577
0.261544079 0.750000000 0.139608577
0.250683278 0.000000000 0.139672890
0.250683278 0.500000000 0.139672890
0.499996394 0.114250422 0.165651828
0.499996394 0.614250422 0.165651828
0.499996394 0.385749578 0.165651858
0.499996394 0.885749519 0.165651858
0.999996483 0.364250392 0.170540452
0.999996483 0.864250422 0.170540452
0.999996483 0.135749578 0.170540452
0.999996483 0.635749578 0.170540452
0.750683308 0.250000000 0.196519375
0.750683308 0.750000000 0.196519375
0.761544108 0.000000000 0.196583688
0.761544108 0.500000000 0.196583688
0.257900923 0.119851977 0.225485489
0.258187681 0.619963944 0.225624025
0.263338745 0.372738540 0.225533620
0.263093621 0.872850537 0.225772291
0.005254438 0.261399418 0.247577235
0.005264429 0.761603653 0.247622922
0.009216673 0.999185145 0.252199262
0.008668380 0.498523951 0.252482772
0.510702491 0.994212925 0.249820963
0.510442019 0.494225025 0.249903172
0.503569484 0.245200828 0.256995887
0.503963411 0.745316029 0.257007003
0.769703865 0.123723410 0.281523645
0.769273579 0.623432636 0.281230986
0.754074514 0.374110103 0.282117695
0.754457295 0.874558091 0.282062322
0.259259343 0.982878506 0.304204196
0.258179128 0.482588261 0.304326117
0.254591376 0.256970435 0.306617230
0.255291075 0.757448852 0.306882560
0.531000376 0.375769943 0.334445268
0.532507837 0.875146747 0.334591687
0.522199810 0.119705155 0.327124566
0.522798002 0.620060921 0.327253819
0.786843240 0.022407632 0.367564887
0.774906099 0.234896541 0.366060048
0.789773583 0.521399796 0.366866708
0.782020390 0.734577954 0.365085125
0.019646060 0.325634480 0.348861039
0.022186859 0.834624410 0.348989189
0.094305724 0.250000000 0.082826398
0.094305724 0.750000000 0.082826398
0.594305754 0.250000000 0.082826398
0.594305754 0.750000000 0.082826398
0.101650499 0.029894177 0.239771202
0.101241395 0.528624594 0.240048259
0.600924850 0.992294312 0.231222421
0.600575686 0.492420375 0.231272727
0.786879003 0.110544018 0.371357441
0.746967494 0.989801526 0.394451708

0.464939445 0.384081692 0.359356701
0.717259884 0.267416269 0.389710426
0.793570936 0.609635174 0.370024353
0.748685777 0.491677284 0.394091457
0.467328787 0.882211626 0.359769732
0.727605402 0.765826583 0.389678895
0.916851878 0.296102196 0.354718000
0.084912047 0.262599140 0.354894876
0.922022760 0.799372256 0.354199857
0.092694625 0.776475847 0.357008219

Hydrated Fh(110) – Fe40O64H8 • 4H2O

1.0

9.2869243622 0.0000000000 0.0000000000
0.0000000000 10.2764081955 0.0000000000
0.0000000000 0.0000000000 31.8661727905

Fe O H
40 68 16

Direct

0.674137771 0.833333373 0.000000000
0.057366032 0.833333313 0.000000000
0.557366073 0.166666687 0.000000000
0.174137741 0.166666687 0.000000000
0.877709568 0.333689868 0.000000000
0.377709448 0.666310132 0.000000000
0.877709568 0.583155096 0.046443813
0.377709448 0.416844964 0.046443813
0.377709448 0.916844845 0.046642952
0.877709568 0.083155155 0.046642952
0.674137771 0.333333373 0.093090288
0.557366073 0.666666627 0.093090288
0.057366032 0.333333313 0.093090288
0.174137741 0.666666687 0.093090288
0.877709568 0.833689809 0.093090288
0.377709448 0.166310191 0.093090288
0.877299726 0.084141284 0.139640108
0.376404077 0.914657056 0.139224723
0.376352578 0.416642934 0.139435589
0.878918290 0.583418965 0.139984995
0.678585768 0.834577560 0.185810283
0.555814803 0.168663129 0.186181828
0.056402784 0.830945313 0.188045010
0.171533287 0.162523329 0.185758561
0.872913837 0.335267276 0.187458441
0.373346061 0.665109098 0.185577080
0.867812514 0.588664711 0.234337747
0.363057286 0.412643045 0.231680915
0.390476555 0.920077920 0.231938362
0.877377033 0.080342762 0.233263716
0.650667310 0.335918605 0.278379887
0.534328401 0.670704722 0.275589764
0.041492481 0.328986973 0.280350327
0.177975267 0.650026560 0.284416825
0.879758894 0.838262379 0.283008337
0.363421142 0.161880165 0.281382322
0.857071280 0.113681413 0.325873762
0.391311765 0.920087457 0.326135576
0.358932495 0.411060244 0.324842036
0.852282822 0.558457971 0.325744957
0.511636436 0.757166386 0.957452476
0.762323320 0.166666687 0.000000000
0.511636436 0.985667229 0.000000000
0.499997169 0.500000000 0.000000000
0.999997199 0.500000000 0.000000000
0.773184121 0.666478097 0.000000000
0.273184061 0.333521903 0.000000000
0.262323260 0.833333313 0.000000000
0.011636457 0.014332831 0.000000000
0.011636457 0.242833614 0.042540543
0.511636436 0.757166386 0.042540543
0.273184061 0.583239079 0.046490721
0.773184121 0.416760981 0.046490721
0.773184121 0.916760862 0.046596043
0.273184061 0.083239138 0.046596043
0.011636457 0.742833614 0.050546281
0.511636436 0.257166386 0.050546281
0.762323320 0.666666627 0.093090288
0.511636436 0.485667229 0.093090288
0.499997169 0.000000000 0.093090288
0.999997199 0.000000000 0.093090288
0.773184121 0.166478157 0.093090288
0.273184061 0.833521843 0.093090288
0.262323260 0.333333313 0.093090288
0.011636457 0.514332771 0.093090288
0.012391875 0.743154764 0.136483848
0.510140002 0.257206678 0.135352209
0.272035420 0.081680700 0.138947055
0.772825420 0.918016732 0.139185369
0.772970438 0.416837215 0.139663979
0.273033917 0.582965314 0.139233172
0.009678627 0.242905349 0.143567890
0.508966267 0.758027792 0.142607138
0.760207474 0.166527197 0.186266065
0.514308989 0.986487746 0.186075896
0.493675381 0.497613341 0.186841518
0.994219184 0.502081096 0.188806713
0.774464190 0.668795168 0.186371431
0.265682280 0.330891937 0.184887514
0.262973130 0.833753884 0.188284516
0.009910538 0.012979344 0.186531544
0.003047165 0.241703033 0.228809878
0.517375946 0.755715549 0.223615915
0.261349440 0.580801904 0.231893703
0.760813117 0.422194839 0.232487187
0.776172340 0.914162695 0.234054968
0.273531735 0.075774685 0.231345236
0.008445282 0.744208694 0.239091471
0.499527991 0.258327246 0.235464603
0.743308306 0.676285565 0.284755886
0.493129343 0.492422551 0.278887302
0.507761300 0.006172221 0.279600799
0.991808534 0.009787146 0.283025861
0.750275314 0.164843872 0.276962876
0.354359627 0.783522129 0.287147194
0.246425688 0.328162163 0.278320730
0.995868027 0.511440277 0.282304972
0.030058032 0.750448942 0.318399727
0.486974478 0.264119923 0.320163041
0.256648749 0.047163695 0.319525391
0.792250216 0.932187557 0.332459092
0.738690436 0.415780753 0.325519204
0.262037128 0.563008964 0.328957289
0.998899281 0.240428373 0.329149544
0.712654948 0.201272473 0.366752505
0.219938591 0.332406938 0.372943848
0.897829175 0.611522734 0.379858285
0.529820144 0.873722553 0.365876257
0.605945766 0.500000000 0.000000000
0.105945729 0.500000000 0.000000000
0.605945766 0.000000000 0.093090288
0.105945729 0.000000000 0.093090288
0.599254906 0.492117941 0.189750880
0.100118078 0.506236374 0.192011595
0.608173251 0.041044313 0.277853042

0.095393613	0.019202650	0.292205930
0.737120569	0.295481771	0.359205544
0.612803578	0.200706661	0.353949219
0.168058649	0.409377068	0.382591784
0.140876591	0.278111517	0.359036028
0.699714005	0.907152534	0.346101582
0.833305061	0.587158859	0.402495295
0.023209639	0.748772860	0.348991096
0.531576514	0.903865278	0.394768327

Hydrated Fh(120) – Fe40O64H8 • 7H2O

1.0

9.2869243622	0.0000000000	0.0000000000
0.0000000000	15.6974725723	0.0000000000
0.0000000000	0.0000000000	27.7125644684

Fe	O	H
40	71	22

Direct

0.866069436	0.895775735	0.010574830
0.045726012	0.395928562	0.010674772
0.662497699	0.395928562	0.010674779
0.366069436	0.788862050	0.022229623
0.366069436	0.288556516	0.022379527
0.866069436	0.074729197	0.045689102
0.866069436	0.574423611	0.045839008
0.162497714	0.967357099	0.057393853
0.545726001	0.967357099	0.057393868
0.366069436	0.467509985	0.057493795
0.866069436	0.252918661	0.080653481
0.045726012	0.753071368	0.080753393
0.662497699	0.753071368	0.080753408
0.366069436	0.146004975	0.092308275
0.366069436	0.645699441	0.092458174
0.866069436	0.431872129	0.115767762
0.866069436	0.931566477	0.115917645
0.162497714	0.324500024	0.127472505
0.545726001	0.324500024	0.127472505
0.366069436	0.824652791	0.127572432
0.865182996	0.611249924	0.151125446
0.044653811	0.112200528	0.147843361
0.659786820	0.108221956	0.149443462
0.364581615	0.503154695	0.161878750
0.378399640	0.002065776	0.156472579
0.872593462	0.791754305	0.187107921
0.874634564	0.297323078	0.192503780
0.155503720	0.680203140	0.199727193
0.545689046	0.681784272	0.197536066
0.346912950	0.177956790	0.201760918
0.889296591	0.964505434	0.230342671
0.015850706	0.462210327	0.218191952
0.671731353	0.477490038	0.229040489
0.373090625	0.836733103	0.239911988
0.378060430	0.362419277	0.232433751
0.854333818	0.140669137	0.249575019
0.857902586	0.651212454	0.255756408
0.207340896	0.026435660	0.278171331
0.543060899	0.030147344	0.261859417
0.356406659	0.538907886	0.263410419
0.499996364	0.493857563	0.999999404
0.999996424	0.000000000	0.004017139
0.261544049	0.895847678	0.010621910
0.250683248	0.395928562	0.010674772
0.761544049	0.788826108	0.022288477
0.761544049	0.288664460	0.022367772
0.999996424	0.675500274	0.030016633
0.988357186	0.181642890	0.034034315
0.488357157	0.181642890	0.034034315
0.499996364	0.687785506	0.038052000
0.261544049	0.074621253	0.045700874
0.261544049	0.574459612	0.045780148
0.750683248	0.967357099	0.057393868
0.761544049	0.467437983	0.057446722
0.499996364	0.363285601	0.064051531
0.999996424	0.869428217	0.068069212
0.499996364	0.851000369	0.070078067
0.999996424	0.357143044	0.074095748
0.261544049	0.252990603	0.080700554
0.250683248	0.753071368	0.080753393
0.761544049	0.145968974	0.092367090
0.761544049	0.645807385	0.092446409
0.999996424	0.032643072	0.100095280
0.988357186	0.538785756	0.104112953
0.488357157	0.538785756	0.104112953
0.499996364	0.044928364	0.108130634
0.261544049	0.431764066	0.115779512
0.261544049	0.931602418	0.115858801
0.750683248	0.324500024	0.127472505
0.761544049	0.824580848	0.127525330
0.499996364	0.720428467	0.134130150
0.995521784	0.228927121	0.140978649
0.497735023	0.208857253	0.140565380
0.001192535	0.713359773	0.144081697
0.260888517	0.608758628	0.150699064
0.248994142	0.104482777	0.152270615
0.760195851	0.503691614	0.162244961
0.757609308	0.004917262	0.160224408
0.009361117	0.388600498	0.164434090
0.996080041	0.899170995	0.173971862
0.481525242	0.895541608	0.177844182
0.496889710	0.399428964	0.177332982
0.258588582	0.790171027	0.187593743
0.262378335	0.287680149	0.187980294
0.749592543	0.683707058	0.196069404
0.732465208	0.201038823	0.205454543
0.492738217	0.077280596	0.202224672
0.993144453	0.578495502	0.209026739
0.494111389	0.565987229	0.209653705
0.975211918	0.081688277	0.207901925
0.376966506	0.953650177	0.265800148
0.230618387	0.459833026	0.224840254
0.782257617	0.863614798	0.234582499
0.836826622	0.393937290	0.234716460
0.000255450	0.736158609	0.238670364
0.991059899	0.242190346	0.250106603
0.506716073	0.246151343	0.246952251
0.505233586	0.752634466	0.248638198
0.244521722	0.135663509	0.255924702
0.250720829	0.636054695	0.257991701
0.740756452	0.039139975	0.264370948
0.757058144	0.555789590	0.270279676
0.492631018	0.439787090	0.269541889
0.034705065	0.974491775	0.279604554
0.891267121	0.127486393	0.327415168
0.272024095	0.055559088	0.348928362
0.507578611	0.114145502	0.314844847
0.267988086	0.494145781	0.332020938
0.753377378	0.743665218	0.296357691
0.230106369	0.789885223	0.291756302
0.228761688	0.314080477	0.294609010
0.094305709	0.181642890	0.034034315
0.594305694	0.181642890	0.034034315
0.094305709	0.538785756	0.104112953
0.594305694	0.538785756	0.104112953
0.099152140	0.888353229	0.168492600

0.587973475	0.895891428	0.175919548
0.078297995	0.209922314	0.240325436
0.608117640	0.230286881	0.227804780
0.910988212	0.065602221	0.326695174
0.980013132	0.154842526	0.338072926
0.290293902	0.003366797	0.366964102
0.372389197	0.081879213	0.340391368
0.507164538	0.210396558	0.276788116
0.592492521	0.117506772	0.335455090
0.172801211	0.516800225	0.339314222
0.258972436	0.431832343	0.329291165
0.648325086	0.738898993	0.288627505
0.775563896	0.798686862	0.276523352
0.248113200	0.726075172	0.286243916
0.129384160	0.793809712	0.279211074
0.262344837	0.255537927	0.300571531
0.132009134	0.302492201	0.279767483

Pu@Fh(100) – Fe40O64H8 • 6H2O Pu(H2O)5

1.0

9.2869243622	0.0000000000	0.0000000000
0.0000000000	11.8661737442	0.0000000000
0.0000000000	0.0000000000	30.1291179657

Fe	O	H	Pu
40	75	30	1

Direct

0.162497729	0.000000000	0.025979901
0.162497729	0.500000000	0.025979901
0.545726061	0.000000000	0.025979908
0.545726061	0.500000000	0.025979908
0.366069466	0.250000030	0.026101509
0.366069466	0.750000000	0.026101509
0.866069496	0.125267372	0.054463953
0.866069496	0.625267386	0.054463953
0.866069496	0.374732584	0.054463953
0.866069496	0.874732614	0.054463953
0.366069466	0.374732584	0.111188836
0.366069466	0.874732614	0.111188836
0.366069466	0.125267401	0.111188836
0.366069466	0.625267386	0.111188836
0.866069496	0.250000000	0.139551282
0.866069496	0.750000000	0.139551282
0.045726035	0.000000000	0.139672890
0.045726035	0.500000000	0.139672890
0.662497759	0.000000000	0.139672890
0.662497759	0.500000000	0.139672890
0.162497729	0.250000000	0.196519375
0.162497729	0.750000000	0.196519375
0.545726061	0.250000000	0.196519375
0.545726061	0.750000000	0.196519375
0.366069466	0.000000000	0.196640968
0.366069466	0.500000000	0.196640968
0.865336776	0.377864212	0.225596935
0.864332259	0.878342092	0.225535572
0.877836883	0.127525628	0.228088140
0.875247478	0.626471877	0.228255525
0.361044884	0.119002946	0.287120998
0.365675807	0.624553740	0.282027662
0.391231447	0.370201021	0.280523032
0.409150809	0.873426080	0.281961441
0.662187994	0.003779307	0.310370922
0.672045231	0.498747528	0.311733663
0.102228604	0.371497631	0.287668258
0.124910876	0.878260493	0.282722265
0.668430269	0.243173227	0.307117939
0.664022148	0.741246343	0.305838585
0.999996483	0.114250407	0.000000963
0.999996483	0.614250422	0.000000963
0.999996483	0.385749578	0.000000970
0.999996483	0.885749519	0.000000970
0.750683308	0.000000000	0.025979908
0.750683308	0.500000000	0.025979908
0.761544108	0.250000000	0.026044222
0.761544108	0.750000000	0.026044222
0.261544079	0.374858558	0.054435298
0.261544079	0.874858558	0.054435298
0.261544079	0.125141427	0.054435298
0.261544079	0.625141442	0.054435298
0.999996483	0.000000000	0.077937789
0.999996483	0.500000000	0.077937789
0.988357246	0.250000000	0.082826398
0.988357246	0.750000000	0.082826398
0.488357216	0.250000000	0.082826398
0.488357216	0.750000000	0.082826398
0.499996394	0.000000000	0.087715007
0.499996394	0.500000000	0.087715007
0.761544108	0.374858558	0.111217491
0.761544108	0.874858558	0.111217491
0.761544108	0.125141427	0.111217491
0.761544108	0.625141442	0.111217491
0.261544079	0.250000000	0.139608577
0.261544079	0.750000000	0.139608577
0.250683278	0.000000000	0.139672890
0.250683278	0.500000000	0.139672890
0.499996394	0.114250422	0.165651828
0.499996394	0.614250422	0.165651828
0.499996394	0.385749578	0.165651858
0.499996394	0.885749519	0.165651858
0.999996483	0.364250392	0.170540452
0.999996483	0.864250422	0.170540452
0.999996483	0.135749578	0.170540452
0.999996483	0.635749578	0.170540452
0.750683308	0.250000000	0.196519375
0.750683308	0.750000000	0.196519375
0.761544108	0.000000000	0.196583688
0.761544108	0.500000000	0.196583688
0.259082764	0.120801091	0.226142555
0.259279519	0.620556474	0.225535959
0.264554113	0.373789072	0.227121174
0.260804415	0.874073327	0.226377174
0.005535428	0.257931679	0.246317789
0.006792791	0.766150951	0.248330459
0.013899649	0.003441308	0.250961542
0.007292992	0.503830969	0.251707345
0.517300487	0.002766513	0.248249173
0.505864024	0.497716427	0.249878153
0.504896283	0.248900324	0.257334620
0.507751703	0.740065217	0.257405490
0.772077203	0.121582091	0.282191753
0.775024712	0.629438877	0.281798273
0.760565162	0.370598048	0.281472087
0.757320642	0.875421345	0.282936424
0.266913027	0.984470248	0.305464059
0.274231225	0.490613848	0.309624076
0.258186936	0.252525002	0.311320186
0.255298853	0.749675870	0.308628261
0.520705223	0.363691956	0.338294148
0.549792767	0.869903743	0.339514047
0.525435865	0.121153913	0.328411669
0.520909309	0.618766010	0.331459820
0.765151918	0.025352350	0.373658061
0.790058136	0.239449769	0.365079254
0.782969713	0.517478704	0.374717653
0.795596123	0.731800258	0.367091775

0.010760476 0.365223914 0.353814870
0.022886556 0.872871876 0.345143139
0.271921843 0.721644521 0.393559664
0.095856942 0.554792047 0.396632016
0.585255861 0.507055640 0.427158564
0.271602720 0.334570706 0.391241699
0.265412152 0.525214851 0.467802972
0.094305724 0.250000000 0.082826398
0.094305724 0.750000000 0.082826398
0.594305754 0.250000000 0.082826398
0.594305754 0.750000000 0.082826398
0.104163036 0.039576940 0.238548100
0.099016778 0.529599667 0.237831935
0.608564556 0.005549944 0.230097771
0.600132644 0.498651832 0.233158812
0.788402796 0.111273415 0.372679293
0.679072559 0.022352681 0.392146111
0.470841229 0.314223200 0.359493196
0.735482156 0.277489305 0.388256341
0.805773199 0.646099269 0.371995062
0.861689568 0.462278366 0.375314951
0.477316856 0.865079761 0.362720966
0.736429811 0.760505497 0.391212374
0.926873744 0.307399750 0.357567519
0.095733814 0.342634380 0.372828394
0.932610393 0.829119027 0.348206013
0.089845024 0.840868711 0.366888553
0.264688164 0.747443318 0.342435062
0.312229484 0.781302452 0.411707610
0.107340477 0.635820746 0.390107274
0.048434466 0.514311075 0.372288764
0.701839268 0.505534887 0.401789337
0.599019766 0.479136974 0.457036614
0.265743077 0.266444147 0.344593018
0.276144832 0.290451467 0.418345630
0.274700165 0.602413535 0.478287160
0.172396541 0.524891555 0.451881528
0.375974536 0.525851190 0.383041650

Pu@Fh(110) – Fe40O64H8 • 4H2O Pu(H2O)5

1.0

9.2869243622 0.0000000000 0.0000000000
0.0000000000 10.2764081955 0.0000000000
0.0000000000 0.0000000000 31.8661727905

Fe O H Pu
40 73 26 1

Direct

0.674137771 0.833333373 0.000000000
0.057366032 0.833333313 0.000000000
0.557366073 0.166666687 0.000000000
0.174137741 0.166666687 0.000000000
0.877709568 0.333689868 0.000000000
0.377709448 0.666310132 0.000000000
0.877709568 0.583155096 0.046443813
0.377709448 0.416844964 0.046443813
0.377709448 0.916844845 0.046642952
0.877709568 0.083155155 0.046642952
0.674137771 0.333333373 0.093090288
0.557366073 0.666666627 0.093090288
0.057366032 0.333333313 0.093090288
0.174137741 0.666666687 0.093090288
0.877709568 0.833689809 0.093090288
0.377709448 0.166310191 0.093090288
0.877891481 0.083430305 0.139584109
0.375279069 0.914716959 0.138591513
0.375691921 0.418338209 0.139826193
0.878365278 0.581947982 0.140087828
0.675822616 0.829827309 0.184584901
0.561875284 0.172999129 0.185067430
0.058796532 0.829522371 0.188399941
0.173779264 0.165490851 0.185882837
0.877567828 0.332801193 0.187030107
0.373606175 0.666092396 0.187426820
0.871984482 0.581590652 0.234779984
0.369677275 0.414119363 0.233511254
0.399625808 0.931742668 0.228348762
0.886242986 0.078330204 0.233737275
0.658716917 0.329652637 0.277653456
0.550402641 0.667162955 0.279074639
0.053046186 0.321005136 0.282056034
0.171214730 0.629902720 0.284397095
0.873696268 0.838520765 0.278043866
0.370155722 0.165356308 0.280313909
0.864564657 0.100986458 0.324112952
0.453328490 0.939556241 0.333208680
0.390124977 0.407808512 0.328089952
0.851906955 0.547624886 0.327175826
0.511636436 0.757166386 0.957452476
0.762323320 0.166666687 0.000000000
0.511636436 0.985667229 0.000000000
0.499997169 0.500000000 0.000000000
0.999997199 0.500000000 0.000000000
0.773184121 0.666478097 0.000000000
0.273184061 0.333521903 0.000000000
0.262323260 0.833333313 0.000000000
0.011636457 0.014332831 0.000000000
0.011636457 0.242833614 0.042540543
0.511636436 0.757166386 0.042540543
0.273184061 0.583239079 0.046490721
0.773184121 0.416760981 0.046490721
0.773184121 0.916760862 0.046596043
0.273184061 0.083239138 0.046596043
0.011636457 0.742833614 0.050546281
0.511636436 0.257166386 0.050546281
0.762323320 0.666666627 0.093090288
0.511636436 0.485667229 0.093090288
0.499997169 0.000000000 0.093090288
0.999997199 0.000000000 0.093090288
0.773184121 0.166478157 0.093090288
0.273184061 0.833521843 0.093090288
0.262323260 0.333333313 0.093090288
0.011636457 0.514332771 0.093090288
0.011498766 0.742643774 0.136777699
0.510567844 0.258578360 0.134890988
0.272534162 0.081756823 0.138985693
0.773203433 0.916031003 0.139046848
0.774705768 0.416119337 0.140147150
0.273009002 0.585537553 0.139676213
0.011947733 0.241803780 0.143926933
0.511199057 0.757665217 0.144000128
0.764578879 0.165647298 0.186186239
0.518152177 0.991044641 0.183492675
0.495458603 0.500005126 0.186609909
0.997358978 0.500655234 0.188649699
0.771200240 0.663976729 0.187475294
0.269920707 0.332123816 0.185398534
0.264544368 0.836345017 0.188057661
0.011407566 0.010069631 0.186356440
0.008536148 0.239553273 0.229399621
0.503741026 0.762230814 0.229102343
0.267419338 0.580230296 0.232780248
0.768141866 0.416330695 0.232871056
0.769286156 0.912290096 0.232177541
0.274554342 0.077610962 0.231703699

0.005970544	0.741747379	0.239448369
0.504389882	0.256540596	0.235235795
0.760466635	0.667902827	0.285586089
0.504289746	0.488589853	0.278026462
0.512589693	0.006788127	0.276518345
0.987391710	0.997284234	0.282508731
0.753809035	0.158134654	0.276468158
0.447573364	0.752273142	0.320310324
0.254709542	0.325876802	0.278767347
0.994856536	0.501899004	0.285340726
0.097323649	0.750757515	0.329456270
0.497031629	0.245772302	0.321588159
0.266541094	0.046811212	0.321049809
0.810197711	0.916587174	0.336737275
0.742100596	0.404758662	0.326277614
0.252972245	0.531782508	0.345087290
0.002927511	0.228942648	0.329554290
0.719822824	0.185990617	0.366589963
0.055778187	0.407431483	0.387280345
0.825967789	0.611807525	0.383821517
0.471332937	0.903638899	0.392529190
0.058412343	0.697971642	0.422690481
0.165522471	0.952129722	0.395374805
0.151145384	0.459256649	0.461141169
0.535881460	0.603531659	0.403110474
0.335338086	0.659982502	0.462771595
0.605945766	0.500000000	0.000000000
0.105945729	0.500000000	0.000000000
0.605945766	0.000000000	0.093090288
0.105945729	0.000000000	0.093090288
0.601472080	0.499403387	0.187320054
0.103447162	0.501685262	0.190143466
0.611532032	0.044606134	0.272710532
0.178103104	0.020958593	0.305549264
0.747118235	0.279307067	0.360342234
0.620650828	0.190941781	0.352063030
0.131703228	0.455901623	0.369621724
0.035401426	0.326529145	0.370491862
0.743057311	0.882125974	0.357418567
0.841479957	0.531334817	0.399656504
0.082360119	0.843474150	0.324599624
0.449030876	0.974003851	0.411809206
0.970076978	0.679052174	0.404933542
0.057910658	0.627979755	0.443525672
0.151739985	0.387537390	0.480912000
0.116320297	0.423399031	0.432567835
0.638058186	0.616961300	0.393999636
0.534226596	0.618248165	0.433345526
0.289680839	0.727269709	0.479562283
0.273736507	0.580264509	0.465919375
0.061129875	0.943452060	0.396090716
0.189861342	0.009467594	0.370993167
0.295306325	0.719783187	0.379791468

Pu@Fh(120) – Fe40O64H8 • 7H2O Pu(H2O)5

1.0

9.2869243622	0.0000000000	0.0000000000
0.0000000000	15.6974725723	0.0000000000
0.0000000000	0.0000000000	27.7125644684

Fe	O	H	Pu
40	76	32	1

Direct

0.866069436	0.895775735	0.010574830
0.045726012	0.395928562	0.010674772
0.662497699	0.395928562	0.010674779
0.366069436	0.788862050	0.022229623
0.366069436	0.288556516	0.022379527
0.866069436	0.074729197	0.045689102
0.866069436	0.574423611	0.045839008
0.162497714	0.967357099	0.057393853
0.545726001	0.967357099	0.057393868
0.366069436	0.467509985	0.057493795
0.866069436	0.252918661	0.080653481
0.045726012	0.753071368	0.080753393
0.662497699	0.753071368	0.080753408
0.366069436	0.146004975	0.092308275
0.366069436	0.645699441	0.092458174
0.866069436	0.431872129	0.115767762
0.866069436	0.931566477	0.115917645
0.162497714	0.324500024	0.127472505
0.545726001	0.324500024	0.127472505
0.366069436	0.824652791	0.127572432
0.861635566	0.607793748	0.150798142
0.047076613	0.110087454	0.150245056
0.658012033	0.112494707	0.148913875
0.367481053	0.503061771	0.161770552
0.374026477	0.004686856	0.155965582
0.869830489	0.783431053	0.183300927
0.863319099	0.291957974	0.190462768
0.159795344	0.683542192	0.196141854
0.551159382	0.684992075	0.197134793
0.364136875	0.186045349	0.200098425
0.856422126	0.973109365	0.220927924
0.045969859	0.468305200	0.212788269
0.668783188	0.462649375	0.225630403
0.364930511	0.845675528	0.242997915
0.376023203	0.361381143	0.233440965
0.853252888	0.143316761	0.251932859
0.880885184	0.629868567	0.253037602
0.180053428	0.043752208	0.267838240
0.531168997	0.039994430	0.262644351
0.372536182	0.535729647	0.265290469
0.499996364	0.493857563	0.999999404
0.999996424	0.000000000	0.004017139
0.261544049	0.895847678	0.010621910
0.250683248	0.395928562	0.010674772
0.761544049	0.788826108	0.022288477
0.761544049	0.288664460	0.022367772
0.999996424	0.675500274	0.030016633
0.988357186	0.181642890	0.034034315
0.488357157	0.181642890	0.034034315
0.499996364	0.687785506	0.038052000
0.261544049	0.074621253	0.045700874
0.261544049	0.574459612	0.045780148
0.750683248	0.967357099	0.057393868
0.761544049	0.467437983	0.057446722
0.499996364	0.363285601	0.064051531
0.999996424	0.869428217	0.068069212
0.499996364	0.851000369	0.070078067
0.999996424	0.357143044	0.074095748
0.261544049	0.252990603	0.080700554
0.250683248	0.753071368	0.080753393
0.761544049	0.145968974	0.092367090
0.761544049	0.645807385	0.092446409
0.999996424	0.032643072	0.100095280
0.988357186	0.538785756	0.104112953
0.488357157	0.538785756	0.104112953
0.499996364	0.044928364	0.108130634
0.261544049	0.431764066	0.115779512

0.261544049	0.931602418	0.115858801
0.750683248	0.324500024	0.127472505
0.761544049	0.824580848	0.127525330
0.499996364	0.720428467	0.134130150
0.998653829	0.223574281	0.139027745
0.499541372	0.209050789	0.141257048
0.001843388	0.715633929	0.144155949
0.262857199	0.611611307	0.153255984
0.250140846	0.107662760	0.153193444
0.762986422	0.501573205	0.162745878
0.755303741	0.000903874	0.162951067
0.997961760	0.382213891	0.168131113
0.985127330	0.895303309	0.178260937
0.477321178	0.898506939	0.177776307
0.497795910	0.403356999	0.177241623
0.253609121	0.795906544	0.190157816
0.264553428	0.291803569	0.185897976
0.753716648	0.681096733	0.197939485
0.753139317	0.179567054	0.197883278
0.490781307	0.078708649	0.201425746
0.005887884	0.587236524	0.205556095
0.500042140	0.571479738	0.211968109
0.995908082	0.070008732	0.216400251
0.382504076	0.959177315	0.269563198
0.250675797	0.466630548	0.223872483
0.779700220	0.854011357	0.240825117
0.745648682	0.353489429	0.230711356
0.995693088	0.733723760	0.239576355
0.986313522	0.243045330	0.247384429
0.496984869	0.258381724	0.247010440
0.509629309	0.763664782	0.247542366
0.259136647	0.152378336	0.255983919
0.277385175	0.650365949	0.261354715
0.732577801	0.032094382	0.264565349
0.794786453	0.530699611	0.264976531
0.495841742	0.441829205	0.272206396
0.020958191	0.959086597	0.289265484
0.806293249	0.165772542	0.321093142
0.267722338	0.065681361	0.348552972
0.526568234	0.142151520	0.308859378
0.260823429	0.515909135	0.330512017
0.822827637	0.682878911	0.314874232
0.226455823	0.809968233	0.299203902
0.233459070	0.310486823	0.290432423
0.870924473	0.032176793	0.367986798
0.739693105	0.884356499	0.350850165
0.199556679	0.896252871	0.380948126
0.047531772	0.612714410	0.363337904
0.985110104	0.792137325	0.398327291
0.094305709	0.181642890	0.034034315
0.594305694	0.181642890	0.034034315
0.094305709	0.538785756	0.104112953
0.594305694	0.538785756	0.104112953
0.089729808	0.884528458	0.175545439
0.581830025	0.903824747	0.172071487
0.079605512	0.218570054	0.237139046
0.596346259	0.279725492	0.239161521
0.844896376	0.089916542	0.351461649
0.843730748	0.220990181	0.331000417
0.330516636	0.017430671	0.355842769
0.335648060	0.110776730	0.338683188
0.506548643	0.195026368	0.285737544
0.629070222	0.153113022	0.319913954
0.176652208	0.551419914	0.341477215
0.242353678	0.455926090	0.337445766
0.723646581	0.669261873	0.322900176
0.678922296	0.833759546	0.245221958
0.363319367	0.688103914	0.259333730
0.238806948	0.747264862	0.298176914
0.250812143	0.246855229	0.284605086
0.131520495	0.313661605	0.280210733
0.967815578	0.990665615	0.314653963
0.917160273	0.045768563	0.398433626
0.768595457	0.944581985	0.358169854
0.651101232	0.887481153	0.332095206
0.158213064	0.949172139	0.368688732
0.229986534	0.864078879	0.350698054
0.952889681	0.627325058	0.348323822
0.060525727	0.655126452	0.388651997
0.064230599	0.835795283	0.402127683
0.898894608	0.812402487	0.414613903
0.957927644	0.813171804	0.304741293