Interaction of Hydrogen with Actinide Dioxide (111) Surfaces (ESI)

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1 Clean Surface

1.1 Fixed Unit Cell Dimensions

Table 1: The fixed unit cell dimensions for the AnO_2 (111) surface.

Surface	Uranium Dioxide			Neptunium Dioxide			Plutonium Dioxide		
(111)	7.742	0.000	0.000	7.697	0.000	0.000	7.651	0.000	0.000
	3.871	6.705	0.000	3.849	6.666	0.000	3.826	6.626	0.000
	0.000	0.000	35.803	0.000	0.000	35.712	0.000	0.000	35.618

1.2 Ionic Positions & Magnetic Structure of the Clean Surface

Table 2: The relaxed ionic direct coordinates for the AnO_2 (111) surface (actinide ions, only).

Actinide Ion	Uranium Dioxide			Neptunium Dioxide			Plutonium Dioxide		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
A	0.667	0.666	0.023	0.667	0.666	0.023	0.667	0.667	0.022
B	0.667	0.167	0.023	0.167	0.166	0.023	0.667	0.166	0.022
C	0.167	0.666	0.023	0.666	0.167	0.023	0.166	0.667	0.022
D	0.167	0.167	0.023	0.167	0.666	0.023	0.166	0.167	0.022
E	0.333	0.333	0.111	0.333	0.333	0.110	0.333	0.333	0.109
F	0.333	0.834	0.111	0.833	0.833	0.110	0.333	0.833	0.109
G	0.833	0.333	0.111	0.333	0.834	0.110	0.834	0.333	0.109
H	0.833	0.833	0.111	0.833	0.333	0.110	0.833	0.833	0.109
I	0.000	1.000	0.199	0.000	0.000	0.199	0.000	0.000	0.197
J	0.000	0.500	0.199	0.500	0.500	0.199	1.000	0.500	0.197
K	0.500	1.000	0.199	1.000	0.500	0.199	0.500	0.000	0.197
L	0.500	0.500	0.199	0.500	0.000	0.199	0.500	0.500	0.197
M	0.667	0.667	0.288	0.667	0.667	0.287	0.667	0.667	0.285
N	0.667	0.166	0.288	0.167	0.167	0.287	0.667	0.167	0.285
O	0.167	0.667	0.288	0.667	0.166	0.287	0.166	0.667	0.285
P	0.167	0.167	0.288	0.167	0.667	0.287	0.167	0.167	0.285
Q	0.333	0.334	0.376	0.333	0.334	0.375	0.333	0.333	0.372
R	0.333	0.833	0.376	0.833	0.834	0.375	0.333	0.834	0.372
S	0.833	0.334	0.376	0.334	0.833	0.375	0.834	0.333	0.372
T	0.833	0.833	0.376	0.833	0.334	0.375	0.834	0.833	0.373

Table 3: The relaxed magnetic vectors for the AnO_2 (111) surface (actinide ions, only).

Actinide Ion	Uranium Dioxide			Neptunium Dioxide			Plutonium Dioxide		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
A	-0.02	-0.34	1.38	-0.50	-1.74	2.02	-0.94	-1.85	-3.21
B	-0.01	-1.22	-0.71	0.63	-2.64	0.03	-0.94	3.71	-0.01
C	-0.04	1.28	0.61	-0.62	-1.26	-2.32	-0.94	-1.86	3.21
D	0.02	1.27	0.64	-0.63	2.64	-0.08	3.71	0.37	-0.74
E	-1.13	-0.38	0.68	-1.07	-1.23	2.15	-1.30	-1.79	-3.09
F	-1.19	-0.33	-0.60	2.70	-0.02	0.00	-1.30	3.57	0.01
G	-0.03	1.24	-0.57	-0.97	-1.27	-2.18	-1.29	-1.79	3.09
H	1.30	-0.38	0.03	-1.00	2.51	0.01	3.80	0.00	0.00
I	-0.64	-0.55	1.06	-0.87	-1.28	2.21	-1.26	-1.79	-3.10
J	0.33	-1.11	-0.75	2.70	-0.02	0.00	-1.26	3.58	0.00
K	-0.95	0.98	0.03	-0.86	-1.28	-2.22	-1.26	-1.79	3.10
L	1.06	0.39	-0.75	-0.86	2.56	-0.02	3.80	0.00	0.00
M	-1.13	-0.38	0.68	-1.07	-1.23	2.15	-1.30	-1.79	-3.09
N	-1.18	-0.33	-0.59	2.70	-0.02	0.00	-1.30	3.57	0.01
O	-0.03	1.24	-0.57	-0.97	-1.27	-2.18	-1.29	-1.79	3.09
P	1.30	-0.38	0.03	-1.00	2.51	0.00	3.80	0.00	0.00
Q	-0.02	-0.34	1.38	-0.50	-1.74	2.02	-0.94	-1.85	-3.21
R	-0.01	-1.22	-0.71	0.63	-2.64	0.03	-0.94	3.71	-0.01
S	-0.04	1.28	0.61	-0.62	-1.26	-2.32	-0.94	-1.86	3.21
T	0.02	1.27	0.64	-0.64	2.63	-0.07	3.71	0.37	-0.73

Note: The magnetic vectors for the low-index AnO_2 (111) surfaces are given for each actinide ion. A diamagnetic (DM) ion (magnetic moment = 0.00), oxygen is not included. An earlier investigation contains a complete analysis of the data.[1]

1.3 K-Point Convergence

The energy of the low-index surfaces has been calculated as function of the number of formula units (**Figure 1**). An earlier investigation contains a complete analysis of the data.[1]

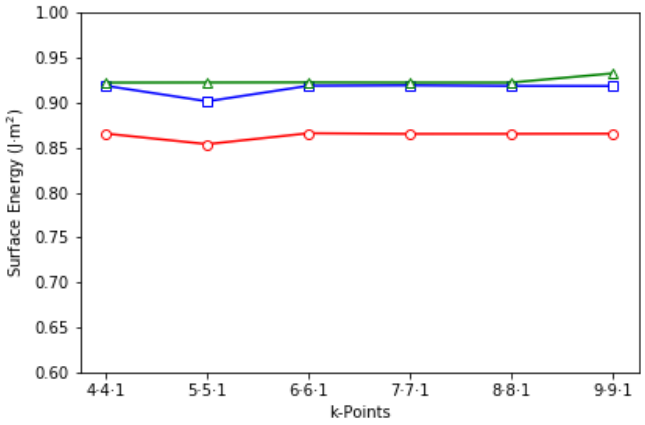

Figure 1: Convergence of the surface energies (J m^{-2}) with respect to the number of formula units (N) employed: (red) uranium dioxide, (blue) neptunium dioxide, and (green) plutonium dioxide.

1.4 Electronic Density of States

The electronic density of states for the clean AnO_2 (An = U, Np, Pu) (111) surface is shown (from noncollinear relativistic PBEsol+U calculations, **Figure 2**).[1]

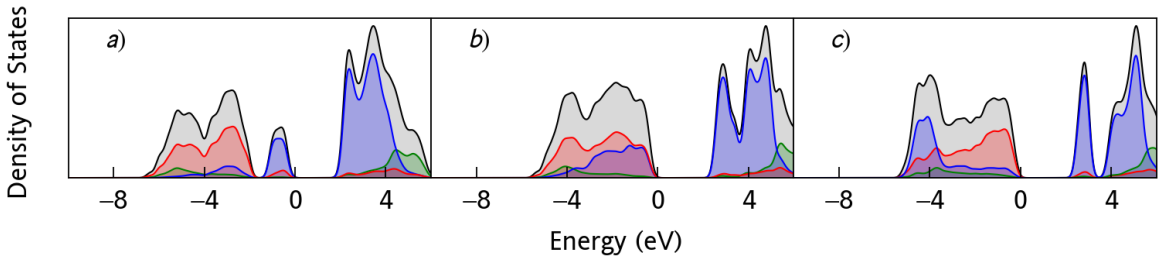

Figure 2: The electronic density of states for the AnO_2 (111) surface, calculated by PBEsol+U: a) UO_2, b) NpO_2, c) PuO_2. The total density of states (black), actinide f- (blue), actinide d- (green), and oxygen p- (red) bands are coloured.[1]

2 Hydrogen Interactions

2.1 Uranium Dioxide

2.1.1 Atomic Hydrogen

Table 4: The ionic positions and magnetic structure of the UO_2 $aH_{(111)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.671	0.664	0.967	0.00	0.00	0.05
	0.329	0.336	0.432	0.00	0.00	0.05
Actinide Ion	0.667	0.666	0.023	-0.01	-0.02	-0.69
	0.668	0.166	0.024	-0.94	-1.01	-0.22
	0.167	0.667	0.024	-0.17	1.35	-0.33
	0.166	0.166	0.024	0.20	-0.19	1.39
	0.333	0.333	0.111	0.91	-0.75	-0.68
	0.333	0.833	0.111	-1.13	-0.48	-0.60
	0.833	0.333	0.111	0.40	1.13	-0.62
	0.833	0.833	0.111	0.03	-0.08	1.35
	0.000	1.000	0.199	1.31	-0.29	-0.24
	0.000	0.500	0.199	-0.89	-1.01	-0.24
	0.500	1.000	0.199	-0.40	1.28	-0.25
	0.500	0.500	0.199	0.00	-0.01	1.35
	0.667	0.667	0.288	0.91	-0.75	-0.68
	0.667	0.167	0.288	-1.13	-0.48	-0.60
	0.167	0.667	0.288	0.40	1.13	-0.62
	0.167	0.167	0.288	0.03	-0.08	1.35
	0.333	0.334	0.376	-0.01	-0.02	-0.69
	0.332	0.834	0.375	-0.94	-1.01	-0.22
	0.833	0.333	0.375	-0.17	1.35	-0.33
	0.834	0.834	0.375	0.20	-0.19	1.39
Oxygen Ion	0.001	0.998	0.003	0.00	-0.01	0.00
	0.502	0.501	0.005	0.01	0.00	0.01
	0.502	0.997	0.005	0.01	0.01	0.01
	0.998	0.501	0.005	0.00	-0.01	0.00
	0.333	0.833	0.046	0.00	0.00	0.00
	0.833	0.833	0.046	0.01	0.00	-0.01
	0.833	0.333	0.046	0.01	0.00	0.00
	0.333	0.334	0.046	0.00	-0.01	0.00
	0.667	0.666	0.087	0.00	-0.01	0.02
	0.166	0.167	0.088	0.00	0.00	-0.01
	0.167	0.668	0.089	0.01	0.00	0.00
	0.666	0.167	0.088	-0.01	0.01	0.00
	0.000	0.500	0.133	-0.01	0.01	0.00
	0.500	0.500	0.133	0.00	0.00	-0.01
	0.499	0.998	0.133	0.01	0.01	0.00
	0.999	0.001	0.133	0.00	-0.01	0.00
	0.334	0.332	0.177	0.00	-0.01	0.01
	0.833	0.833	0.177	0.00	0.00	-0.01
	0.834	0.335	0.177	0.01	0.00	0.01
	0.332	0.834	0.178	-0.01	0.00	0.00
	0.668	0.166	0.221	-0.01	0.00	0.00
	0.167	0.167	0.222	0.00	0.00	-0.01
	0.166	0.665	0.221	0.01	0.00	0.00
	0.666	0.668	0.221	0.00	-0.01	0.00
	0.001	0.999	0.266	0.00	-0.01	0.00
	0.500	0.500	0.266	0.00	0.00	-0.01
	0.501	0.002	0.266	0.01	0.01	0.00
	1.000	0.500	0.266	-0.01	0.01	0.00
	0.334	0.833	0.310	-0.01	0.01	0.00
	0.834	0.833	0.311	0.00	0.00	-0.01
	0.833	0.332	0.310	0.01	0.00	0.00
	0.333	0.334	0.312	0.00	-0.01	0.02
	0.667	0.666	0.352	0.00	-0.01	0.01
	0.167	0.167	0.353	0.00	0.00	-0.01
	0.167	0.667	0.353	0.01	0.00	0.00
	0.667	0.167	0.353	0.00	0.00	0.00
	0.002	0.499	0.393	0.00	0.00	0.00
	0.498	0.499	0.394	0.01	0.00	0.01
	0.498	0.003	0.393	0.01	0.01	0.01
	0.999	0.002	0.395	0.00	-0.01	0.00

Table 5: The ionic positions and magnetic structure of the UO_2 $bH_{(111)}$ configuration.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.500	0.500	0.963	0.00	0.00	0.00
	0.500	0.500	0.436	0.00	0.00	0.00
Actinide Ion	0.672	0.673	0.024	1.39	-0.31	-0.53
	0.673	0.155	0.024	-0.95	-1.05	-0.54
	0.155	0.672	0.024	-0.44	1.36	-0.54
	0.166	0.168	0.022	-0.08	0.00	-2.44
	0.333	0.334	0.110	0.95	-0.42	-0.91
	0.334	0.833	0.110	-0.95	-0.63	-0.77
	0.833	0.334	0.110	-0.11	0.88	-1.06
	0.833	0.833	0.112	0.02	0.02	1.34
	0.000	1.000	0.199	1.31	-0.35	-0.20
	0.000	0.500	0.199	-0.94	-0.91	-0.37
	0.500	1.000	0.199	-0.14	1.31	-0.31
	0.500	0.500	0.199	0.34	-0.32	1.28
	0.667	0.666	0.288	0.95	-0.42	-0.91
	0.666	0.167	0.288	-0.95	-0.63	-0.77
	0.167	0.666	0.288	-0.11	0.88	-1.06
	0.167	0.167	0.287	0.02	0.02	1.34
	0.328	0.327	0.375	1.39	-0.31	-0.53
	0.327	0.845	0.375	-0.95	-1.05	-0.54
	0.845	0.328	0.375	-0.43	1.36	-0.54
	0.834	0.832	0.377	-0.08	0.00	-2.43
Oxygen Ion	0.992	0.989	0.001	0.01	-0.01	0.02
	0.500	0.500	0.990	0.00	0.00	0.00
	0.519	0.993	0.001	0.00	0.01	0.02
	0.988	0.520	0.001	-0.01	-0.01	0.02
	0.346	0.811	0.044	-0.01	0.00	0.02
	0.833	0.834	0.047	0.00	0.00	-0.01
	0.812	0.343	0.044	0.01	0.01	0.02
	0.343	0.346	0.044	0.00	-0.01	0.02
	0.669	0.668	0.089	0.00	-0.01	0.00
	0.167	0.166	0.087	0.00	0.00	0.02
	0.165	0.669	0.089	0.01	0.00	0.01
	0.666	0.165	0.089	-0.01	0.01	0.01
	0.002	0.497	0.133	-0.01	0.01	0.00
	0.500	0.501	0.133	0.00	0.00	-0.01
	0.498	0.000	0.133	0.01	0.00	0.00
	0.000	0.001	0.133	0.00	-0.01	0.00
	0.335	0.332	0.177	0.00	-0.01	0.01
	0.834	0.833	0.178	0.00	0.00	-0.01
	0.834	0.335	0.177	0.01	0.01	0.01
	0.333	0.833	0.178	-0.01	0.01	0.00
	0.667	0.167	0.221	-0.01	0.01	0.00
	0.166	0.167	0.221	0.00	0.00	-0.01
	0.166	0.665	0.222	0.01	0.01	0.01
	0.665	0.668	0.221	0.00	-0.01	0.01
	1.000	0.999	0.266	0.00	-0.01	0.00
	0.500	0.499	0.266	0.00	0.00	0.00
	0.502	1.000	0.266	0.01	0.00	0.01
	0.998	0.503	0.266	-0.01	0.01	0.01
	0.334	0.835	0.310	-0.01	0.01	0.01
	0.833	0.834	0.312	0.00	0.00	0.01
	0.835	0.331	0.310	0.01	0.00	0.00
	0.331	0.332	0.310	0.00	-0.01	0.00
	0.657	0.654	0.355	0.00	-0.01	0.02
	0.167	0.166	0.351	0.00	0.00	-0.01
	0.188	0.657	0.355	0.01	0.01	0.02
	0.654	0.189	0.355	-0.01	0.00	0.02
	0.012	0.480	0.398	-0.01	0.00	0.02
	0.500	0.500	0.408	0.00	0.00	-0.01
	0.481	0.007	0.398	0.00	0.01	0.02
	0.008	0.011	0.398	0.01	-0.01	0.02

2.1.2 Molecular Hydrogen

Table 6: The ionic positions and magnetic structure of the UO_2 $aH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.601	0.649	0.947	0.00	0.00	0.00
	0.604	0.747	0.946	0.00	0.00	0.00
	0.399	0.351	0.452	0.00	0.00	0.00
	0.396	0.253	0.452	0.00	0.00	0.00
Actinide Ion	0.666	0.667	0.023	1.21	-0.65	-0.30
	0.666	0.168	0.023	-1.07	-0.87	-0.29
	0.166	0.667	0.023	-0.30	1.35	-0.27
	0.166	0.167	0.023	-0.10	0.08	1.41
	0.333	0.333	0.111	0.90	-0.73	-0.73
	0.334	0.833	0.111	-1.27	-0.21	-0.82
	0.833	0.334	0.111	0.20	1.25	-0.87
	0.833	0.833	0.111	0.00	0.02	1.36
	0.000	1.000	0.199	1.17	-0.53	-0.45
	0.000	0.500	0.199	-1.07	-0.72	-0.41
	0.500	1.000	0.199	-0.25	1.29	-0.35
	0.500	0.500	0.199	0.02	0.05	1.35
	0.667	0.667	0.288	0.90	-0.73	-0.73
	0.666	0.167	0.288	-1.27	-0.21	-0.82
	0.167	0.666	0.288	0.20	1.25	-0.87
	0.167	0.167	0.288	0.00	0.02	1.36
	0.334	0.333	0.376	1.21	-0.65	-0.30
	0.334	0.832	0.376	-1.07	-0.87	-0.29
	0.834	0.333	0.376	-0.30	1.35	-0.26
	0.834	0.833	0.376	-0.10	0.08	1.41
Oxygen Ion	0.999	0.001	0.002	0.01	-0.01	0.00
	0.499	0.499	0.002	0.00	0.00	0.00
	0.499	0.004	0.002	0.01	0.01	0.00
	0.999	0.501	0.002	-0.01	0.00	0.00
	0.335	0.833	0.045	-0.01	0.00	0.00
	0.833	0.833	0.046	0.00	0.00	-0.01
	0.833	0.333	0.046	0.01	0.00	0.00
	0.333	0.334	0.046	0.00	-0.01	0.00
	0.667	0.666	0.088	0.00	-0.01	0.00
	0.167	0.166	0.088	0.00	0.00	-0.01
	0.167	0.667	0.088	0.01	0.00	0.00
	0.666	0.168	0.088	-0.01	0.01	0.00
	0.001	0.500	0.133	-0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	-0.01
	0.500	1.000	0.133	0.01	0.00	0.00
	1.000	0.000	0.133	0.00	-0.01	0.00
	0.335	0.333	0.178	0.00	-0.01	0.01
	0.832	0.833	0.177	0.00	0.00	-0.01
	0.835	0.334	0.177	0.01	0.00	0.01
	0.331	0.834	0.177	-0.01	0.00	0.01
	0.669	0.166	0.221	-0.01	0.00	0.00
	0.168	0.167	0.222	0.00	0.00	-0.01
	0.165	0.666	0.221	0.01	0.00	0.01
	0.665	0.667	0.221	0.00	-0.01	0.00
	0.000	1.000	0.266	0.00	-0.01	0.00
	0.500	0.500	0.266	0.00	0.00	0.00
	0.500	0.000	0.266	0.01	0.00	0.00
	0.999	0.500	0.266	-0.01	0.01	0.01
	0.334	0.832	0.311	-0.01	0.00	0.00
	0.833	0.834	0.311	0.00	0.00	-0.01
	0.833	0.333	0.311	0.01	0.00	0.00
	0.333	0.334	0.311	0.00	-0.01	0.00
	0.667	0.666	0.353	0.00	-0.01	0.00
	0.167	0.167	0.353	0.00	0.00	-0.01
	0.167	0.667	0.353	0.01	0.00	0.00
	0.665	0.167	0.353	-0.01	0.00	0.00
	0.001	0.499	0.397	-0.01	0.00	0.00
	0.501	0.501	0.397	0.00	0.00	0.00
	0.501	0.996	0.397	0.008	0.011	-0.004
	0.001	0.999	0.397	0.006	-0.009	-0.003

Table 7: The ionic positions and magnetic structure of the UO_2 $bH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.642	0.706	0.945	0.00	0.00	0.00
	0.611	0.627	0.948	0.00	0.00	0.00
	0.358	0.294	0.454	0.00	0.00	0.00
	0.389	0.373	0.451	0.00	0.00	0.00
Actinide Ion	0.667	0.666	0.023	1.21	-0.68	-0.24
	0.667	0.166	0.023	-1.03	-0.92	-0.26
	0.166	0.666	0.023	-0.28	1.35	-0.24
	0.167	0.166	0.023	-0.08	0.07	1.41
	0.333	0.333	0.111	0.44	-1.02	-0.90
	0.334	0.833	0.111	-1.20	-0.12	-0.90
	0.833	0.333	0.111	0.38	1.08	-0.91
	0.833	0.833	0.111	0.04	0.03	1.35
	0.000	1.000	0.199	1.16	-0.54	-0.44
	0.000	0.500	0.199	-1.07	-0.71	-0.42
	0.500	1.000	0.199	-0.15	1.29	-0.39
	0.500	0.500	0.199	0.03	0.01	1.34
	0.667	0.667	0.288	0.44	-1.02	-0.90
	0.666	0.167	0.288	-1.20	-0.12	-0.90
	0.167	0.667	0.288	0.38	1.09	-0.91
	0.167	0.167	0.288	0.04	0.03	1.35
	0.333	0.334	0.376	1.21	-0.68	-0.24
	0.333	0.834	0.376	-1.03	-0.92	-0.26
	0.834	0.334	0.376	-0.28	1.35	-0.24
	0.833	0.834	0.376	-0.08	0.07	1.41
Oxygen Ion	0.000	0.998	0.002	0.01	-0.01	0.00
	0.500	0.497	0.002	0.00	0.00	0.00
	0.499	1.000	0.002	0.01	0.01	0.00
	1.000	0.499	0.002	-0.01	0.00	0.00
	0.334	0.832	0.046	-0.01	0.00	0.00
	0.833	0.833	0.046	0.00	0.00	-0.01
	0.833	0.333	0.046	0.01	0.01	0.00
	0.333	0.333	0.046	0.00	-0.01	0.01
	0.667	0.665	0.088	0.00	-0.01	0.00
	0.167	0.166	0.088	0.00	0.00	-0.01
	0.167	0.667	0.088	0.01	0.00	0.00
	0.666	0.167	0.088	-0.01	0.01	0.00
	0.001	0.500	0.133	-0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	0.00
	0.500	1.000	0.133	0.01	0.01	0.00
	1.000	0.001	0.133	0.00	-0.01	0.00
	0.335	0.333	0.177	0.00	-0.01	0.01
	0.832	0.834	0.177	0.00	0.00	-0.01
	0.835	0.334	0.177	0.01	0.00	0.01
	0.331	0.834	0.177	-0.01	0.00	0.01
	0.669	0.166	0.221	-0.01	0.00	0.01
	0.168	0.166	0.222	0.00	0.00	-0.01
	0.165	0.666	0.221	0.01	0.00	0.01
	0.665	0.667	0.221	0.00	-0.01	0.01
	0.000	0.999	0.266	0.00	-0.01	0.00
	0.500	0.500	0.266	0.00	0.00	0.00
	0.500	0.000	0.266	0.01	0.01	0.00
	0.999	0.500	0.266	-0.01	0.01	0.00
	0.334	0.833	0.311	-0.01	0.01	0.00
	0.833	0.834	0.311	0.00	0.00	-0.01
	0.833	0.333	0.311	0.01	0.00	0.00
	0.333	0.335	0.311	0.00	-0.01	0.00
	0.667	0.667	0.353	0.00	-0.01	0.01
	0.167	0.167	0.353	0.00	0.00	-0.01
	0.167	0.667	0.353	0.01	0.01	0.01
	0.666	0.168	0.353	-0.01	0.00	0.01
	0.000	0.501	0.397	-0.01	0.00	0.00
	0.500	0.503	0.397	0.00	0.00	0.00
	0.501	0.000	0.397	0.007	0.011	-0.004
	1.000	0.002	0.397	0.006	-0.009	-0.003

Table 8: The ionic positions and magnetic structure of the UO_2 $cH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.500	0.500	0.933	0.00	0.00	0.00
	0.500	0.500	0.911	0.00	0.00	0.00
	0.500	0.500	0.487	0.00	0.00	0.00
	0.500	0.500	0.466	0.00	0.00	0.00
Actinide Ion	0.667	0.666	0.023	1.26	-0.48	-0.36
	0.668	0.166	0.023	-1.04	-0.87	-0.34
	0.167	0.666	0.023	-0.21	1.34	-0.31
	0.167	0.166	0.023	0.03	-0.08	1.41
	0.333	0.333	0.111	0.81	-0.81	-0.76
	0.333	0.833	0.111	-1.08	-0.40	-0.73
	0.833	0.333	0.111	0.45	1.05	-0.84
	0.833	0.833	0.111	-0.01	0.01	1.35
	0.000	1.000	0.199	1.21	-0.46	-0.40
	0.000	0.500	0.199	-0.99	-0.82	-0.41
	0.500	1.000	0.199	-0.35	1.27	-0.29
	0.500	0.500	0.199	-0.02	0.02	1.35
	0.667	0.667	0.288	0.81	-0.81	-0.76
	0.667	0.167	0.288	-1.08	-0.40	-0.73
	0.167	0.667	0.288	0.45	1.05	-0.84
	0.167	0.167	0.288	-0.01	0.01	1.35
	0.333	0.334	0.376	1.26	-0.48	-0.36
	0.332	0.834	0.376	-1.04	-0.88	-0.34
	0.833	0.334	0.376	-0.21	1.34	-0.31
	0.833	0.834	0.376	0.03	-0.08	1.41
Oxygen Ion	0.002	0.997	0.002	0.01	-0.01	0.00
	0.501	0.499	0.002	0.00	0.00	0.00
	0.502	1.000	0.002	0.01	0.01	0.00
	0.000	0.499	0.002	-0.01	0.00	0.00
	0.334	0.833	0.046	-0.01	0.00	0.00
	0.833	0.833	0.046	0.00	0.00	-0.01
	0.833	0.333	0.046	0.01	0.00	0.01
	0.333	0.333	0.046	0.00	-0.01	0.00
	0.667	0.666	0.088	0.00	-0.01	0.00
	0.167	0.166	0.088	0.00	0.00	-0.01
	0.167	0.667	0.088	0.01	0.00	0.00
	0.666	0.167	0.088	-0.01	0.01	0.00
	0.001	0.500	0.133	-0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	-0.01
	0.500	1.000	0.133	0.01	0.00	0.00
	1.000	0.000	0.133	0.00	-0.01	0.00
	0.333	0.332	0.177	0.00	-0.01	0.01
	0.832	0.834	0.177	0.00	0.00	-0.01
	0.834	0.335	0.177	0.01	0.00	0.01
	0.331	0.834	0.177	-0.01	0.01	0.01
	0.669	0.166	0.221	-0.01	0.00	0.00
	0.168	0.166	0.222	0.00	0.00	-0.01
	0.166	0.665	0.221	0.01	0.00	0.01
	0.667	0.668	0.221	0.00	-0.01	0.01
	0.000	1.000	0.266	0.00	-0.01	0.00
	0.500	0.500	0.266	0.00	0.00	-0.01
	0.500	0.000	0.266	0.01	0.01	0.00
	0.999	0.500	0.266	-0.01	0.01	0.00
	0.334	0.833	0.311	-0.01	0.01	0.00
	0.833	0.834	0.311	0.00	0.00	-0.01
	0.833	0.333	0.311	0.01	0.00	0.00
	0.333	0.334	0.311	0.00	-0.01	0.00
	0.667	0.667	0.353	0.00	-0.01	0.01
	0.167	0.167	0.353	0.00	0.00	-0.01
	0.167	0.667	0.353	0.01	0.00	0.01
	0.666	0.167	0.353	-0.01	0.00	0.00
	1.000	0.501	0.397	-0.01	0.00	0.00
	0.499	0.501	0.397	0.00	0.00	0.00
	0.498	0.000	0.397	0.005	0.01	-0.002
	0.998	0.003	0.397	0.005	-0.009	-0.002

Table 9: The ionic positions and magnetic structure of the UO_2 $dH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.327	0.829	0.938	0.00	0.00	0.00
	0.338	0.837	0.917	0.00	0.00	0.00
	0.662	0.163	0.482	0.00	0.00	0.00
	0.673	0.171	0.461	0.00	0.00	0.00
Actinide Ion	0.666	0.666	0.023	1.30	-0.46	-0.28
	0.667	0.166	0.023	-1.01	-0.95	-0.24
	0.166	0.666	0.023	-0.28	1.35	-0.27
	0.166	0.166	0.023	-0.01	-0.02	1.41
	0.333	0.333	0.111	0.79	-0.79	-0.80
	0.333	0.833	0.111	-1.04	-0.39	-0.80
	0.833	0.333	0.111	0.16	1.17	-0.68
	0.833	0.833	0.111	0.00	0.00	1.35
	0.000	1.000	0.199	1.23	-0.46	-0.36
	0.000	0.500	0.199	-0.92	-0.96	-0.29
	0.500	1.000	0.199	-0.20	1.27	-0.43
	0.500	0.500	0.199	0.02	0.01	1.35
	0.667	0.667	0.288	0.79	-0.79	-0.80
	0.667	0.167	0.288	-1.04	-0.39	-0.80
	0.167	0.667	0.288	0.16	1.17	-0.68
	0.167	0.167	0.288	0.00	0.00	1.35
	0.334	0.334	0.376	1.30	-0.46	-0.28
	0.333	0.834	0.376	-1.01	-0.96	-0.24
	0.834	0.334	0.376	-0.28	1.35	-0.27
	0.834	0.834	0.376	-0.01	-0.02	1.41
Oxygen Ion	0.000	0.998	0.002	0.01	-0.01	0.00
	0.500	0.499	0.002	0.00	0.00	0.00
	0.500	0.998	0.002	0.01	0.01	0.00
	0.999	0.499	0.002	-0.01	0.00	0.00
	0.333	0.833	0.046	-0.01	0.00	0.00
	0.834	0.833	0.046	0.00	0.00	-0.01
	0.833	0.333	0.046	0.01	0.00	0.00
	0.333	0.333	0.046	0.00	-0.01	0.00
	0.667	0.665	0.088	0.00	-0.01	0.00
	0.167	0.166	0.088	0.00	0.00	-0.01
	0.167	0.667	0.088	0.01	0.00	0.00
	0.666	0.167	0.088	-0.01	0.01	0.00
	0.000	0.500	0.133	-0.01	0.01	0.00
	0.500	0.500	0.133	0.00	0.00	-0.01
	0.500	0.999	0.133	0.01	0.00	0.00
	0.999	0.001	0.133	0.00	-0.01	0.00
	0.335	0.331	0.177	0.00	-0.01	0.01
	0.834	0.832	0.177	0.00	0.00	-0.01
	0.833	0.335	0.178	0.01	0.00	0.01
	0.331	0.835	0.177	-0.01	0.00	0.01
	0.669	0.165	0.221	-0.01	0.00	0.01
	0.166	0.168	0.222	0.00	0.00	-0.01
	0.167	0.665	0.221	0.01	0.00	0.00
	0.665	0.669	0.221	0.00	-0.01	0.01
	0.001	0.999	0.266	0.00	-0.01	0.00
	0.500	0.500	0.266	0.00	0.00	-0.01
	0.500	0.001	0.266	0.01	0.01	0.00
	1.000	0.500	0.266	-0.01	0.01	0.00
	0.334	0.833	0.311	-0.01	0.01	0.00
	0.833	0.834	0.311	0.00	0.00	-0.01
	0.833	0.333	0.311	0.01	0.00	0.00
	0.333	0.335	0.311	0.00	-0.01	0.00
	0.667	0.667	0.353	0.00	-0.01	0.01
	0.166	0.167	0.353	0.00	0.00	-0.01
	0.167	0.667	0.353	0.01	0.01	0.00
	0.667	0.167	0.353	-0.01	0.00	0.01
	0.001	0.501	0.397	-0.01	0.00	0.00
	0.500	0.501	0.397	0.00	0.00	0.00
	0.500	0.002	0.396	0.004	0.01	-0.003
	1.000	0.002	0.397	0.005	-0.009	-0.003

Table 10: The ionic positions and magnetic structure of the UO_2 $eH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.395	0.707	0.941	0.00	0.00	0.00
	0.348	0.798	0.928	0.00	0.00	0.00
	0.605	0.293	0.458	0.00	0.00	0.00
	0.652	0.202	0.471	0.00	0.00	0.00
Actinide Ion	0.666	0.668	0.023	1.35	-0.41	-0.13
	0.666	0.167	0.023	-1.06	-0.92	-0.12
	0.166	0.667	0.023	-0.43	1.35	-0.09
	0.167	0.167	0.023	-0.04	-0.06	1.42
	0.333	0.334	0.111	0.79	-0.57	-0.96
	0.333	0.833	0.111	-1.03	-0.25	-0.88
	0.833	0.334	0.111	0.64	0.80	-0.98
	0.833	0.834	0.111	0.00	0.09	1.35
	0.000	1.000	0.199	1.20	-0.47	-0.43
	0.000	0.500	0.199	-1.08	-0.73	-0.39
	0.500	1.000	0.199	-0.43	1.28	-0.21
	0.500	0.500	0.199	0.15	0.11	1.34
	0.667	0.666	0.288	0.79	-0.57	-0.96
	0.667	0.167	0.288	-1.03	-0.25	-0.88
	0.167	0.666	0.288	0.64	0.80	-0.98
	0.167	0.166	0.288	0.00	0.09	1.35
	0.334	0.332	0.376	1.35	-0.41	-0.13
	0.334	0.833	0.376	-1.06	-0.92	-0.12
	0.834	0.333	0.376	-0.43	1.35	-0.09
	0.833	0.833	0.376	-0.04	-0.06	1.42
Oxygen Ion	0.998	0.001	0.002	0.01	-0.01	0.00
	0.499	0.501	0.002	0.00	0.00	0.00
	0.500	0.002	0.002	0.01	0.01	0.00
	0.999	0.500	0.002	-0.01	0.00	0.00
	0.334	0.834	0.045	-0.01	0.00	0.00
	0.833	0.833	0.046	0.00	0.00	-0.01
	0.833	0.333	0.046	0.01	0.01	0.00
	0.333	0.334	0.046	0.00	-0.01	0.00
	0.666	0.667	0.088	0.00	-0.01	0.00
	0.167	0.166	0.088	0.00	0.00	-0.01
	0.167	0.667	0.088	0.01	0.00	0.00
	0.666	0.168	0.088	-0.01	0.01	0.00
	0.000	0.500	0.133	-0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	0.00
	0.499	0.000	0.133	0.01	0.00	0.00
	1.000	1.000	0.133	0.00	-0.01	0.00
	0.334	0.334	0.178	0.00	-0.01	0.01
	0.832	0.834	0.177	0.00	0.00	-0.01
	0.835	0.334	0.177	0.01	0.01	0.01
	0.332	0.833	0.178	-0.01	0.00	0.01
	0.668	0.167	0.221	-0.01	0.00	0.01
	0.168	0.166	0.222	0.00	0.00	-0.01
	0.165	0.666	0.221	0.01	0.00	0.01
	0.666	0.666	0.221	0.00	-0.01	0.01
	0.000	0.000	0.266	0.00	-0.01	0.00
	0.500	0.500	0.266	0.00	0.00	0.00
	0.501	1.000	0.266	0.01	0.00	0.00
	1.000	0.500	0.266	-0.01	0.01	0.01
	0.334	0.832	0.311	-0.01	0.01	0.00
	0.833	0.834	0.311	0.00	0.00	-0.01
	0.833	0.333	0.311	0.01	0.00	0.00
	0.334	0.333	0.311	0.00	-0.01	0.00
	0.667	0.666	0.353	0.00	-0.01	0.01
	0.167	0.167	0.353	0.00	0.00	-0.01
	0.167	0.667	0.353	0.00	0.01	0.01
	0.666	0.166	0.353	-0.01	0.00	0.00
	0.001	0.500	0.397	-0.01	0.00	-0.01
	0.501	0.499	0.397	0.00	0.00	-0.01
	0.500	0.998	0.397	0.005	0.01	-0.005
	0.002	0.999	0.397	0.007	-0.008	-0.005

2.2 Neptunium Dioxide

2.2.1 Atomic Hydrogen

Table 11: The ionic positions and magnetic structure of the NpO_2 $aH_{(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.500	0.500	0.962	0.00	0.00	0.00
	0.500	0.500	0.435	0.00	0.00	0.00
Actinide Ion	0.672	0.672	0.023	2.42	-1.06	-0.63
	0.167	0.167	0.021	1.49	1.01	3.20
	0.672	0.155	0.023	-2.13	-1.56	-0.63
	0.155	0.672	0.023	-0.26	2.64	-0.62
	0.333	0.333	0.110	2.21	-1.22	-0.97
	0.833	0.833	0.112	-0.03	0.00	2.70
	0.333	0.833	0.110	-2.17	-1.32	-0.92
	0.833	0.333	0.110	-0.12	2.54	-0.92
	0.000	0.000	0.199	2.21	-1.32	-0.82
	0.500	0.500	0.199	0.00	-0.01	2.69
	1.000	0.500	0.199	-0.44	-0.28	-2.64
	0.500	0.000	0.199	-0.05	2.54	-0.91
	0.667	0.667	0.287	2.21	-1.22	-0.97
	0.167	0.167	0.286	-0.03	0.00	2.70
	0.667	0.167	0.287	-2.17	-1.32	-0.92
	0.167	0.667	0.287	-0.12	2.54	-0.91
	0.328	0.328	0.374	2.42	-1.07	-0.63
	0.833	0.833	0.376	1.49	1.01	3.20
	0.328	0.845	0.374	-2.13	-1.56	-0.63
	0.845	0.328	0.374	-0.26	2.63	-0.62
Oxygen Ion	0.993	0.987	0.000	0.01	-0.02	0.00
	0.987	0.520	0.000	-0.03	-0.01	0.00
	0.500	0.500	0.990	0.00	0.00	0.00
	0.520	0.993	0.000	0.00	0.02	0.00
	0.347	0.811	0.044	-0.02	0.00	0.00
	0.811	0.341	0.044	0.01	0.01	0.01
	0.833	0.833	0.047	0.00	0.00	-0.01
	0.341	0.347	0.044	0.00	-0.01	0.01
	0.671	0.665	0.089	0.00	-0.01	0.00
	0.665	0.164	0.089	-0.01	0.01	0.00
	0.167	0.167	0.087	-0.01	0.00	-0.01
	0.164	0.671	0.089	0.01	0.00	0.00
	0.003	0.497	0.133	-0.01	0.00	0.01
	0.497	0.999	0.132	0.01	0.00	0.00
	0.500	0.500	0.132	0.00	0.00	-0.01
	0.999	0.003	0.132	0.00	-0.01	0.00
	0.336	0.331	0.177	-0.01	-0.01	0.01
	0.331	0.834	0.177	-0.01	0.01	0.00
	0.833	0.833	0.177	0.00	0.00	0.00
	0.834	0.336	0.177	0.00	0.00	0.01
	0.669	0.166	0.221	-0.01	0.00	0.00
	0.166	0.664	0.221	0.00	0.00	0.01
	0.167	0.167	0.221	0.00	0.00	-0.01
	0.664	0.669	0.221	-0.01	-0.01	0.01
	0.001	0.997	0.265	0.00	-0.01	0.00
	0.997	0.503	0.265	-0.01	0.00	0.01
	0.500	0.500	0.265	0.00	0.00	-0.01
	0.503	0.001	0.265	0.01	0.00	0.00
	0.335	0.836	0.309	-0.01	0.01	0.00
	0.836	0.329	0.309	0.01	0.00	0.00
	0.833	0.833	0.310	-0.01	0.00	-0.01
	0.329	0.335	0.309	0.00	-0.01	0.00
	0.659	0.653	0.354	0.00	-0.01	0.01
	0.653	0.189	0.354	-0.02	0.00	0.01
	0.167	0.167	0.350	0.00	0.00	-0.01
	0.189	0.659	0.354	0.01	0.01	0.01
	0.013	0.480	0.397	-0.03	-0.01	0.00
	0.480	0.007	0.397	0.00	0.02	0.00
	0.500	0.500	0.408	0.00	0.00	0.00
	0.007	0.013	0.397	0.01	-0.02	0.00

2.2.2 Molecular Hydrogen

Table 12: The ionic positions and magnetic structure of the NpO_2 $aH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.619	0.643	0.946	0.00	0.00	0.00
	0.617	0.744	0.947	0.00	0.00	0.00
	0.381	0.357	0.451	0.00	0.00	0.00
	0.383	0.256	0.451	0.00	0.00	0.00
Actinide Ion	0.667	0.667	0.022	2.27	-1.36	-0.61
	0.167	0.168	0.023	0.06	0.11	2.66
	0.667	0.167	0.023	-2.27	-1.34	-0.63
	0.168	0.667	0.023	0.06	2.64	-0.62
	0.333	0.333	0.110	2.18	-1.26	-0.98
	0.833	0.834	0.110	0.01	-0.01	2.70
	0.334	0.833	0.110	-2.17	-1.28	-0.96
	0.834	0.334	0.110	-0.01	2.51	-0.98
	0.000	0.000	0.199	2.68	0.02	0.04
	0.500	0.500	0.199	-0.01	-0.02	2.35
	1.000	0.500	0.199	-2.21	-1.28	-0.87
	0.500	0.000	0.199	-0.01	2.56	-0.87
	0.667	0.667	0.287	2.18	-1.26	-0.98
	0.167	0.166	0.287	0.01	-0.01	2.70
	0.666	0.167	0.287	-2.17	-1.28	-0.96
	0.166	0.666	0.287	-0.01	2.51	-0.98
	0.333	0.333	0.375	2.27	-1.36	-0.61
	0.833	0.832	0.375	0.06	0.10	2.66
	0.333	0.833	0.374	-2.27	-1.34	-0.63
	0.832	0.333	0.375	0.07	2.64	-0.62
Oxygen Ion	0.003	0.000	0.001	0.01	-0.01	0.00
	0.999	0.503	0.002	-0.02	0.00	0.00
	0.500	0.498	0.001	0.00	0.00	0.01
	0.501	0.002	0.001	0.01	0.01	0.00
	0.336	0.832	0.045	-0.01	0.00	0.00
	0.833	0.333	0.045	0.01	0.01	0.00
	0.833	0.835	0.045	0.00	0.00	-0.01
	0.332	0.334	0.045	0.00	-0.01	0.00
	0.668	0.665	0.088	0.00	-0.01	0.00
	0.664	0.169	0.088	-0.01	0.01	0.00
	0.167	0.166	0.087	0.00	0.00	-0.01
	0.168	0.668	0.088	0.01	0.00	0.00
	0.003	0.499	0.132	-0.01	0.00	0.00
	0.499	0.999	0.132	0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	0.00
	0.999	0.002	0.132	0.00	-0.01	0.00
	0.335	0.330	0.177	0.00	-0.01	0.01
	0.330	0.835	0.177	-0.01	0.00	0.00
	0.833	0.833	0.176	-0.01	0.00	-0.01
	0.835	0.335	0.177	0.01	0.00	0.01
	0.670	0.165	0.220	-0.01	0.00	0.00
	0.165	0.665	0.220	0.01	0.00	0.00
	0.167	0.167	0.221	0.00	0.00	-0.01
	0.665	0.670	0.220	0.00	-0.01	0.01
	0.001	0.998	0.265	0.00	-0.01	0.00
	0.997	0.501	0.265	-0.01	0.01	0.00
	0.500	0.500	0.264	0.00	0.00	0.00
	0.501	0.001	0.265	0.01	0.00	0.00
	0.336	0.831	0.310	-0.01	0.00	0.00
	0.832	0.332	0.310	0.01	0.00	0.00
	0.833	0.834	0.310	0.00	0.00	-0.01
	0.332	0.335	0.310	0.00	-0.01	0.00
	0.668	0.666	0.352	0.00	-0.01	0.00
	0.664	0.168	0.353	-0.01	0.00	0.00
	0.167	0.165	0.352	0.00	0.00	-0.01
	0.167	0.667	0.352	0.01	0.01	0.00
	0.001	0.497	0.396	-0.02	0.00	0.00
	0.499	0.998	0.396	0.01	0.02	0.00
	0.500	0.502	0.396	0.00	0.00	0.00
	0.997	1.000	0.396	0.01	-0.01	0.00

Table 13: The ionic positions and magnetic structure of the NpO_2 $bH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.670	0.671	0.945	0.00	0.00	0.00
	0.614	0.614	0.950	0.00	0.00	0.00
	0.330	0.329	0.453	0.00	0.00	0.00
	0.386	0.386	0.448	0.00	0.00	0.00
Actinide Ion	0.668	0.665	0.022	2.27	-1.37	-0.57
	0.168	0.165	0.023	0.00	-0.22	2.65
	0.667	0.166	0.023	-2.29	-1.31	-0.62
	0.167	0.665	0.023	0.02	2.64	-0.63
	0.334	0.333	0.110	2.18	-1.25	-0.97
	0.833	0.833	0.110	0.02	0.00	2.70
	0.333	0.833	0.110	-2.19	-1.25	-0.96
	0.834	0.333	0.110	0.00	2.53	-0.95
	0.000	0.000	0.199	2.29	-1.09	-0.73
	0.500	0.500	0.199	-0.10	0.02	2.70
	1.000	0.500	0.199	-2.21	-1.28	-0.87
	0.500	0.000	0.199	-0.02	2.56	-0.85
	0.666	0.667	0.287	2.18	-1.25	-0.97
	0.167	0.167	0.287	0.02	0.00	2.70
	0.667	0.167	0.287	-2.19	-1.25	-0.96
	0.166	0.667	0.287	0.00	2.53	-0.95
	0.332	0.335	0.375	2.27	-1.37	-0.57
	0.832	0.835	0.374	0.00	-0.22	2.65
	0.333	0.834	0.374	-2.29	-1.31	-0.62
	0.833	0.335	0.374	0.02	2.63	-0.64
Oxygen Ion	0.002	0.996	0.002	0.01	-0.01	0.00
	0.002	0.496	0.002	-0.02	0.00	0.00
	0.499	0.498	0.001	0.00	0.00	0.00
	0.503	1.000	0.002	0.01	0.02	0.00
	0.335	0.834	0.045	-0.01	0.00	0.00
	0.832	0.333	0.045	0.01	0.01	0.00
	0.834	0.832	0.046	0.00	0.00	-0.01
	0.333	0.335	0.045	0.00	-0.01	0.00
	0.668	0.663	0.088	0.00	-0.01	0.00
	0.665	0.167	0.088	-0.01	0.01	0.00
	0.166	0.167	0.087	0.00	0.00	-0.01
	0.169	0.667	0.088	0.01	0.00	0.00
	0.003	0.499	0.132	-0.01	0.00	0.00
	0.499	0.999	0.132	0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	-0.01
	0.999	0.002	0.132	0.00	-0.01	0.00
	0.335	0.330	0.177	0.00	-0.01	0.00
	0.331	0.835	0.177	-0.01	0.00	0.00
	0.833	0.833	0.176	0.00	0.00	-0.01
	0.835	0.335	0.177	0.01	0.00	0.00
	0.669	0.165	0.220	-0.01	0.00	0.00
	0.165	0.665	0.220	0.01	0.00	0.00
	0.167	0.167	0.221	0.00	0.00	-0.01
	0.665	0.670	0.220	0.00	-0.01	0.00
	0.001	0.998	0.265	0.00	-0.01	0.00
	0.997	0.501	0.265	-0.01	0.00	0.00
	0.500	0.500	0.264	0.00	0.00	-0.01
	0.501	0.001	0.265	0.01	0.00	0.00
	0.335	0.833	0.309	-0.01	0.00	0.00
	0.831	0.333	0.309	0.01	0.00	0.00
	0.834	0.833	0.310	0.00	0.00	-0.01
	0.332	0.337	0.310	0.00	-0.01	0.00
	0.667	0.665	0.352	0.00	-0.01	0.00
	0.665	0.166	0.352	-0.01	0.01	0.00
	0.166	0.168	0.352	0.00	0.00	-0.01
	0.168	0.667	0.352	0.01	0.01	0.00
	0.998	0.504	0.396	-0.02	0.00	0.00
	0.497	0.000	0.395	0.01	0.02	0.00
	0.501	0.502	0.396	0.00	0.00	0.00
	0.998	0.004	0.396	0.01	-0.01	0.00

Table 14: The ionic positions and magnetic structure of the NpO_2 $cH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.500	0.501	0.932	0.00	0.00	0.00
	0.500	0.501	0.910	0.00	0.00	0.00
	0.500	0.499	0.487	0.00	0.00	0.00
	0.500	0.499	0.465	0.00	0.00	0.00
Actinide Ion	0.667	0.666	0.023	2.26	-1.35	-0.63
	0.167	0.166	0.023	-0.01	-0.15	2.66
	0.667	0.166	0.023	-2.30	-1.29	-0.64
	0.167	0.666	0.023	0.01	2.63	-0.65
	0.333	0.333	0.110	2.18	-1.25	-0.97
	0.833	0.833	0.110	0.00	-0.01	2.70
	0.333	0.833	0.110	-2.19	-1.26	-0.96
	0.834	0.333	0.110	-0.01	2.52	-0.97
	0.000	0.000	0.199	2.20	-1.29	-0.88
	0.500	0.500	0.199	0.06	0.05	2.69
	1.000	0.500	0.199	-2.14	-1.40	-0.87
	0.500	0.000	0.199	0.02	2.55	-0.89
	0.667	0.667	0.287	2.18	-1.25	-0.97
	0.167	0.167	0.287	0.00	-0.01	2.70
	0.667	0.167	0.287	-2.19	-1.26	-0.96
	0.166	0.667	0.287	-0.01	2.52	-0.97
	0.333	0.334	0.374	2.26	-1.35	-0.63
	0.833	0.834	0.375	0.00	-0.16	2.66
	0.333	0.834	0.375	-2.30	-1.29	-0.65
	0.833	0.334	0.374	0.02	2.63	-0.66
Oxygen Ion	0.002	0.996	0.002	0.01	-0.02	0.00
	0.998	0.498	0.002	-0.02	0.00	0.00
	0.500	0.500	0.001	0.00	0.00	0.01
	0.502	0.001	0.002	0.01	0.02	0.00
	0.336	0.834	0.045	-0.01	0.00	0.00
	0.832	0.331	0.045	0.01	0.01	0.00
	0.834	0.833	0.046	0.00	0.00	-0.01
	0.332	0.336	0.045	0.00	-0.01	0.00
	0.668	0.663	0.088	0.00	-0.01	0.00
	0.664	0.168	0.088	-0.01	0.01	0.00
	0.167	0.167	0.087	0.00	0.00	-0.01
	0.169	0.668	0.088	0.01	0.00	0.00
	0.003	0.499	0.132	-0.01	0.00	0.00
	0.499	0.998	0.132	0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	-0.01
	0.999	0.002	0.132	0.00	-0.01	0.00
	0.335	0.330	0.177	0.00	-0.01	0.00
	0.330	0.835	0.177	-0.01	0.00	0.00
	0.833	0.833	0.176	0.00	0.00	-0.01
	0.835	0.335	0.177	0.01	0.01	0.00
	0.670	0.165	0.220	-0.01	0.00	0.00
	0.165	0.665	0.220	0.01	0.01	0.00
	0.167	0.167	0.221	0.00	0.00	-0.01
	0.665	0.670	0.220	0.00	-0.01	0.00
	0.001	0.998	0.265	0.00	-0.01	0.00
	0.997	0.501	0.265	-0.01	0.01	0.00
	0.500	0.500	0.264	0.00	0.00	-0.01
	0.501	0.002	0.265	0.01	0.00	0.00
	0.336	0.832	0.309	-0.01	0.00	0.00
	0.831	0.332	0.310	0.01	0.00	0.00
	0.833	0.833	0.310	0.00	0.00	-0.01
	0.332	0.337	0.310	0.00	-0.01	0.00
	0.668	0.664	0.352	0.00	-0.01	0.00
	0.664	0.166	0.352	-0.01	0.01	0.00
	0.166	0.167	0.352	0.00	0.00	-0.01
	0.168	0.669	0.352	0.01	0.01	0.00
	0.002	0.502	0.395	-0.02	0.00	0.00
	0.498	0.999	0.396	0.01	0.02	0.00
	0.500	0.500	0.396	0.00	0.00	0.01
	0.998	0.004	0.396	0.01	-0.01	0.00

Table 15: The ionic positions and magnetic structure of the NpO_2 $dH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.557	0.551	0.913	0.00	0.00	0.00
	0.536	0.533	0.933	0.00	0.00	0.00
	0.443	0.449	0.484	0.00	0.00	0.00
	0.464	0.467	0.464	0.00	0.00	0.00
Actinide Ion	0.667	0.666	0.023	2.26	-1.34	-0.66
	0.168	0.166	0.023	0.04	-0.04	2.66
	0.667	0.166	0.023	-2.28	-1.31	-0.66
	0.167	0.666	0.023	0.00	2.63	-0.65
	0.333	0.333	0.110	2.17	-1.25	-1.00
	0.834	0.833	0.110	0.00	-0.01	2.70
	0.333	0.833	0.110	-2.19	-1.27	-0.95
	0.834	0.333	0.110	0.00	2.53	-0.94
	0.000	0.000	0.199	2.43	-0.97	-0.64
	0.500	0.500	0.199	-0.01	-0.01	2.70
	1.000	0.500	0.199	-2.09	-1.54	-0.70
	0.500	0.000	0.199	-0.05	2.55	-0.88
	0.667	0.667	0.287	2.17	-1.25	-1.00
	0.166	0.167	0.287	0.00	-0.01	2.70
	0.667	0.167	0.287	-2.19	-1.27	-0.95
	0.166	0.667	0.287	0.00	2.53	-0.94
	0.333	0.334	0.374	2.26	-1.35	-0.66
	0.832	0.834	0.374	0.04	-0.04	2.66
	0.333	0.834	0.374	-2.28	-1.31	-0.66
	0.833	0.334	0.374	0.00	2.63	-0.65
Oxygen Ion	0.003	0.997	0.002	0.01	-0.02	0.00
	0.998	0.499	0.002	-0.02	0.00	0.00
	0.499	0.500	0.001	0.00	0.00	0.01
	0.502	0.001	0.002	0.01	0.02	0.00
	0.336	0.833	0.045	-0.01	0.00	0.00
	0.832	0.332	0.045	0.01	0.01	0.00
	0.834	0.833	0.046	0.00	0.00	-0.01
	0.332	0.334	0.046	0.00	-0.01	0.00
	0.668	0.664	0.088	0.00	-0.01	0.00
	0.666	0.167	0.088	-0.01	0.01	0.00
	0.166	0.166	0.088	0.00	0.00	-0.01
	0.168	0.667	0.088	0.01	0.00	0.00
	0.001	0.500	0.132	-0.01	0.00	0.00
	0.499	0.998	0.132	0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	-0.01
	0.999	0.002	0.132	0.00	-0.01	0.00
	0.335	0.330	0.177	0.00	-0.01	0.00
	0.331	0.834	0.177	-0.01	0.00	0.00
	0.833	0.833	0.176	0.00	0.00	-0.01
	0.834	0.335	0.177	0.01	0.00	0.00
	0.669	0.166	0.220	-0.01	0.00	0.00
	0.166	0.665	0.220	0.01	0.00	0.00
	0.167	0.167	0.221	0.00	0.00	-0.01
	0.665	0.670	0.221	0.00	-0.01	0.00
	0.001	0.998	0.265	0.00	-0.01	0.00
	0.999	0.500	0.265	-0.01	0.01	0.00
	0.500	0.500	0.264	0.00	0.00	-0.01
	0.501	0.002	0.265	0.01	0.00	0.00
	0.334	0.833	0.309	-0.01	0.00	0.00
	0.832	0.333	0.309	0.01	0.00	0.00
	0.834	0.834	0.310	0.00	0.00	-0.01
	0.332	0.336	0.310	0.00	-0.01	0.00
	0.668	0.666	0.352	0.00	-0.01	0.00
	0.664	0.167	0.352	-0.01	0.00	0.00
	0.166	0.167	0.352	0.00	0.00	-0.01
	0.168	0.668	0.352	0.01	0.01	0.00
	0.002	0.501	0.395	-0.02	0.00	0.00
	0.498	0.999	0.396	0.01	0.02	0.00
	0.501	0.500	0.396	0.00	0.00	0.01
	0.997	0.003	0.395	0.01	-0.01	0.00

Table 16: The ionic positions and magnetic structure of the NpO_2 $eH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.409	0.691	0.940	0.00	0.00	0.00
	0.368	0.779	0.926	0.00	0.00	0.00
	0.632	0.221	0.471	0.00	0.00	0.00
	0.591	0.309	0.458	0.00	0.00	0.00
Actinide Ion	0.665	0.667	0.023	2.28	-1.33	-0.64
	0.165	0.168	0.023	-0.15	0.08	2.66
	0.665	0.168	0.023	-2.32	-1.27	-0.62
	0.166	0.667	0.023	0.02	2.64	-0.62
	0.333	0.334	0.110	2.18	-1.25	-0.97
	0.833	0.834	0.110	0.00	0.00	2.70
	0.333	0.834	0.110	-2.18	-1.26	-0.97
	0.833	0.333	0.110	0.00	2.52	-0.96
	0.000	0.000	0.199	2.20	-1.29	-0.88
	0.500	0.500	0.199	0.00	0.00	2.70
	1.000	0.500	0.199	-2.21	-1.27	-0.88
	0.500	0.000	0.199	-0.01	2.55	-0.90
	0.667	0.666	0.287	2.18	-1.25	-0.97
	0.167	0.166	0.287	0.00	0.00	2.70
	0.667	0.166	0.287	-2.18	-1.26	-0.97
	0.167	0.667	0.287	0.00	2.52	-0.96
	0.335	0.333	0.374	2.28	-1.33	-0.64
	0.835	0.832	0.375	-0.15	0.08	2.66
	0.335	0.832	0.374	-2.31	-1.27	-0.62
	0.834	0.333	0.374	0.02	2.64	-0.62
Oxygen Ion	0.000	0.997	0.002	0.01	-0.02	0.00
	0.996	0.502	0.002	-0.02	0.00	0.00
	0.500	0.500	0.001	0.00	0.00	0.01
	0.498	0.005	0.002	0.01	0.01	0.00
	0.335	0.832	0.045	-0.01	0.00	0.00
	0.833	0.332	0.045	0.01	0.01	0.00
	0.833	0.833	0.046	0.00	0.00	-0.01
	0.331	0.337	0.045	0.00	-0.01	0.00
	0.667	0.664	0.088	0.00	-0.01	0.00
	0.663	0.169	0.088	-0.01	0.01	0.00
	0.167	0.167	0.087	0.00	0.00	-0.01
	0.167	0.669	0.088	0.01	0.00	0.00
	0.002	0.499	0.132	-0.01	0.00	0.00
	0.499	0.999	0.132	0.01	0.00	0.00
	0.500	0.500	0.133	0.00	0.00	-0.01
	0.998	0.003	0.132	0.00	-0.01	0.00
	0.335	0.330	0.177	0.00	-0.01	0.00
	0.330	0.835	0.177	-0.01	0.01	0.00
	0.833	0.833	0.176	0.00	0.00	-0.01
	0.835	0.335	0.177	0.01	0.01	0.00
	0.670	0.165	0.220	-0.01	0.00	0.00
	0.165	0.665	0.220	0.01	0.00	0.00
	0.167	0.167	0.221	0.00	0.00	-0.01
	0.665	0.670	0.220	0.00	-0.01	0.00
	0.002	0.997	0.265	0.00	-0.01	0.00
	0.998	0.501	0.265	-0.01	0.00	0.00
	0.500	0.500	0.264	0.00	0.00	-0.01
	0.501	0.001	0.265	0.01	0.00	0.00
	0.337	0.831	0.310	-0.01	0.00	0.00
	0.833	0.331	0.309	0.01	0.00	0.00
	0.833	0.833	0.310	0.00	0.00	-0.01
	0.333	0.336	0.310	0.00	-0.01	0.00
	0.669	0.663	0.352	0.00	-0.01	0.00
	0.665	0.168	0.352	-0.01	0.00	0.00
	0.167	0.167	0.352	0.00	0.00	-0.01
	0.167	0.668	0.352	0.01	0.01	0.00
	0.004	0.498	0.396	-0.02	0.00	0.00
	0.502	0.995	0.395	0.01	0.02	0.00
	0.500	0.500	0.396	0.00	0.00	0.00
	1.000	0.003	0.395	0.01	-0.02	0.00

2.3 Plutonium Dioxide

2.3.1 Atomic Hydrogen

Table 17: The ionic positions and magnetic structure of the PuO_2 $aH_{(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.667	0.667	0.955	0.28	0.16	-0.01
	0.333	0.333	0.440	0.28	0.16	-0.01
Actinide Ion	0.667	0.667	0.022	-3.23	-1.86	-0.63
	0.667	0.166	0.022	0.01	3.71	-0.93
	0.166	0.667	0.022	3.22	-1.85	-0.93
	0.166	0.167	0.022	-0.07	-0.02	3.79
	0.333	0.333	0.109	-3.08	-1.78	-1.32
	0.333	0.833	0.109	0.00	3.56	-1.31
	0.833	0.333	0.109	3.09	-1.79	-1.31
	0.833	0.833	0.109	0.00	0.00	3.80
	0.000	0.000	0.197	-3.10	-1.79	-1.27
	1.000	0.500	0.197	0.00	3.58	-1.27
	0.500	0.000	0.197	3.10	-1.79	-1.27
	0.500	0.500	0.197	0.00	0.00	3.80
	0.667	0.667	0.285	-3.08	-1.78	-1.32
	0.667	0.167	0.285	0.00	3.57	-1.31
	0.167	0.667	0.285	3.09	-1.79	-1.31
	0.167	0.167	0.285	0.00	0.00	3.80
	0.333	0.333	0.372	-3.23	-1.86	-0.63
	0.333	0.834	0.372	0.01	3.71	-0.93
	0.834	0.333	0.372	3.22	-1.85	-0.93
	0.834	0.833	0.372	-0.06	-0.02	3.79
Oxygen Ion	0.999	1.000	0.001	-0.02	-0.01	-0.02
	0.500	0.500	0.001	0.03	0.02	0.02
	0.001	0.499	0.001	0.03	0.04	-0.02
	0.499	0.001	0.001	0.05	0.01	-0.02
	0.333	0.834	0.045	0.00	0.00	-0.01
	0.834	0.333	0.045	0.00	0.00	-0.01
	0.833	0.833	0.044	0.00	0.00	0.00
	0.333	0.333	0.045	0.00	0.00	-0.01
	0.667	0.667	0.087	0.01	0.01	0.00
	0.167	0.167	0.087	0.00	0.00	0.01
	0.667	0.167	0.087	0.00	0.00	0.00
	0.166	0.667	0.087	0.00	0.00	0.00
	0.000	0.500	0.131	0.00	0.00	0.00
	0.500	0.000	0.131	0.00	0.00	0.00
	0.500	0.500	0.131	0.00	0.00	0.00
	1.000	1.000	0.131	0.00	0.00	0.00
	0.333	0.333	0.175	0.00	0.00	0.00
	0.833	0.833	0.175	0.00	0.00	0.00
	0.333	0.833	0.175	0.00	0.00	0.00
	0.833	0.333	0.175	0.00	0.00	0.00
	0.667	0.167	0.219	0.00	0.00	0.00
	0.167	0.667	0.219	0.00	0.00	0.00
	0.167	0.167	0.219	0.00	0.00	0.00
	0.667	0.667	0.219	0.00	0.00	0.00
	0.000	0.000	0.263	0.00	0.00	0.00
	0.500	0.500	0.263	0.00	0.00	0.00
	1.000	0.500	0.263	0.00	0.00	0.00
	0.500	1.000	0.263	0.00	0.00	0.00
	0.333	0.833	0.308	0.00	0.00	0.00
	0.834	0.333	0.308	0.00	0.00	0.00
	0.833	0.833	0.307	0.00	0.00	0.01
	0.333	0.333	0.307	0.01	0.01	0.00
	0.667	0.667	0.350	0.00	0.00	-0.01
	0.167	0.167	0.350	0.00	0.00	0.00
	0.667	0.166	0.350	0.00	0.00	-0.01
	0.166	0.667	0.350	0.00	0.00	-0.01
	0.999	0.501	0.394	0.03	0.04	-0.02
	0.501	0.999	0.394	0.05	0.01	-0.02
	0.500	0.500	0.394	0.03	0.02	0.02
	0.001	0.000	0.394	-0.02	-0.01	-0.02

Table 18: The ionic positions and magnetic structure of the PuO_2 $bH_{(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.500	0.500	0.963	0.00	0.00	0.00
	0.500	0.500	0.432	0.00	0.00	0.00
Actinide Ion	0.673	0.673	0.023	-3.01	-1.74	-1.52
	0.673	0.154	0.023	0.00	3.48	-1.52
	0.155	0.673	0.023	3.01	-1.74	-1.52
	0.167	0.167	0.020	0.00	0.00	4.81
	0.333	0.333	0.109	-3.07	-1.77	-1.36
	0.333	0.833	0.109	0.00	3.54	-1.37
	0.833	0.333	0.109	3.07	-1.77	-1.37
	0.833	0.833	0.111	0.00	0.00	3.80
	0.000	0.000	0.197	-3.09	-1.79	-1.29
	1.000	0.500	0.197	0.00	3.57	-1.29
	0.500	0.000	0.197	3.09	-1.79	-1.29
	0.500	0.500	0.197	0.00	0.00	3.80
	0.667	0.667	0.286	-3.07	-1.77	-1.36
	0.667	0.167	0.286	0.00	3.54	-1.37
	0.167	0.667	0.286	3.07	-1.77	-1.37
	0.167	0.167	0.284	0.00	0.00	3.80
	0.327	0.327	0.372	-3.01	-1.74	-1.52
	0.327	0.846	0.372	0.00	3.48	-1.52
	0.845	0.327	0.372	3.01	-1.74	-1.52
	0.833	0.833	0.374	0.00	0.00	4.81
Oxygen Ion	0.990	0.990	0.999	-0.02	-0.01	0.00
	0.500	0.500	0.990	0.00	0.00	0.02
	0.990	0.520	0.999	0.00	0.02	0.00
	0.521	0.990	0.999	0.02	-0.01	0.00
	0.343	0.814	0.043	0.00	0.00	0.01
	0.814	0.343	0.043	0.00	0.00	0.01
	0.833	0.833	0.047	0.00	0.00	0.00
	0.343	0.343	0.043	0.00	0.00	0.01
	0.668	0.668	0.087	0.00	0.00	0.00
	0.167	0.167	0.087	0.00	0.00	0.00
	0.668	0.163	0.087	0.00	0.00	0.00
	0.163	0.668	0.087	0.00	0.00	0.00
	0.001	0.499	0.132	0.00	0.00	0.00
	0.499	0.000	0.132	0.00	0.00	0.00
	0.500	0.500	0.131	0.00	0.00	0.00
	0.001	0.000	0.132	0.00	0.00	0.00
	0.334	0.334	0.175	0.00	0.00	0.00
	0.833	0.833	0.176	0.00	0.00	0.00
	0.334	0.833	0.175	0.00	0.00	0.00
	0.832	0.334	0.175	0.00	0.00	0.00
	0.666	0.167	0.220	0.00	0.00	0.00
	0.168	0.666	0.220	0.00	0.00	0.00
	0.167	0.167	0.219	0.00	0.00	0.00
	0.666	0.666	0.220	0.00	0.00	0.00
	0.999	1.000	0.263	0.00	0.00	0.00
	0.500	0.500	0.264	0.00	0.00	0.00
	0.999	0.501	0.263	0.00	0.00	0.00
	0.501	1.000	0.263	0.00	0.00	0.00
	0.332	0.837	0.307	0.00	0.00	0.00
	0.837	0.332	0.307	0.00	0.00	0.00
	0.833	0.833	0.308	0.00	0.00	0.00
	0.332	0.332	0.307	0.00	0.00	0.00
	0.657	0.657	0.352	0.00	0.00	0.01
	0.167	0.167	0.348	0.00	0.00	0.00
	0.657	0.186	0.352	0.00	0.00	0.01
	0.186	0.657	0.352	0.00	0.00	0.01
	0.010	0.480	0.395	0.00	0.02	0.00
	0.479	0.010	0.395	0.02	-0.01	0.00
	0.500	0.500	0.404	0.00	0.00	0.02
	0.010	0.010	0.395	-0.02	-0.01	0.00

2.3.2 Molecular Hydrogen

Table 19: The ionic positions and magnetic structure of the PuO_2 $aH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.621	0.640	0.946	0.00	0.00	0.00
	0.623	0.739	0.945	0.00	0.00	0.00
	0.379	0.360	0.449	0.00	0.00	0.00
	0.377	0.261	0.449	0.00	0.00	0.00
Actinide Ion	0.665	0.668	0.022	-3.19	-1.82	-1.06
	0.665	0.168	0.023	0.01	3.72	-0.90
	0.164	0.668	0.023	3.22	-1.85	-0.92
	0.164	0.168	0.022	-0.01	0.02	3.79
	0.332	0.334	0.110	-3.09	-1.79	-1.30
	0.332	0.834	0.109	0.00	3.57	-1.30
	0.832	0.334	0.109	3.09	-1.78	-1.31
	0.832	0.834	0.110	0.00	0.00	3.80
	0.000	0.000	0.197	-3.10	-1.79	-1.26
	1.000	0.500	0.197	0.00	3.58	-1.26
	0.500	0.000	0.197	3.10	-1.79	-1.28
	0.500	0.500	0.197	0.00	0.00	3.80
	0.668	0.666	0.285	-3.09	-1.79	-1.30
	0.668	0.166	0.285	0.00	3.57	-1.30
	0.168	0.666	0.285	3.09	-1.78	-1.31
	0.168	0.166	0.285	0.00	0.00	3.80
	0.335	0.332	0.373	-3.19	-1.82	-1.06
	0.335	0.832	0.372	0.02	3.72	-0.90
	0.836	0.332	0.372	3.22	-1.85	-0.92
	0.836	0.832	0.372	-0.01	0.02	3.79
Oxygen Ion	0.997	0.001	0.001	-0.02	-0.01	-0.02
	0.497	0.500	0.001	0.00	0.00	0.02
	0.998	0.501	0.001	0.00	0.02	-0.01
	0.498	0.003	0.001	0.02	-0.01	-0.01
	0.331	0.835	0.044	0.00	0.00	-0.01
	0.832	0.335	0.045	0.00	0.00	-0.01
	0.831	0.834	0.045	0.00	0.00	0.00
	0.330	0.334	0.045	0.00	0.00	-0.01
	0.665	0.668	0.087	0.00	0.00	0.00
	0.165	0.167	0.087	0.00	0.00	0.01
	0.665	0.167	0.087	0.00	0.00	0.00
	0.165	0.668	0.087	0.00	0.00	0.00
	0.999	0.501	0.131	0.00	0.00	0.00
	0.499	0.001	0.131	0.00	0.00	0.00
	0.499	0.500	0.131	0.00	0.00	0.00
	0.999	0.000	0.131	0.00	0.00	0.00
	0.333	0.333	0.175	0.00	0.00	0.00
	0.833	0.833	0.175	0.00	0.00	0.00
	0.333	0.834	0.175	0.00	0.00	0.00
	0.833	0.334	0.175	0.00	0.00	0.00
	0.667	0.166	0.219	0.00	0.00	0.00
	0.167	0.666	0.219	0.00	0.00	0.00
	0.167	0.167	0.219	0.00	0.00	0.00
	0.667	0.667	0.219	0.00	0.00	0.00
	0.001	1.000	0.263	0.00	0.00	0.00
	0.501	0.500	0.263	0.00	0.00	0.00
	0.001	0.499	0.263	0.00	0.00	0.00
	0.501	0.999	0.263	0.00	0.00	0.00
	0.335	0.833	0.308	0.00	0.00	0.00
	0.835	0.332	0.308	0.00	0.00	0.00
	0.835	0.833	0.307	0.00	0.00	0.01
	0.335	0.332	0.308	0.00	0.00	0.00
	0.670	0.666	0.350	0.00	0.00	-0.01
	0.169	0.166	0.350	0.00	0.00	0.00
	0.669	0.165	0.350	0.00	0.00	-0.01
	0.168	0.665	0.350	0.00	0.00	-0.01
	0.002	0.499	0.394	0.00	0.02	-0.01
	0.502	0.997	0.394	0.02	-0.01	-0.01
	0.503	0.500	0.394	0.00	0.00	0.02
	0.003	0.999	0.394	-0.02	-0.01	-0.02

Table 20: The ionic positions and magnetic structure of the PuO_2 $bH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.676	0.676	0.944	0.00	0.00	0.00
	0.619	0.619	0.948	0.00	0.00	0.00
	0.324	0.324	0.451	0.00	0.00	0.00
	0.381	0.381	0.447	0.00	0.00	0.00
Actinide Ion	0.668	0.668	0.022	-3.17	-1.83	-1.10
	0.668	0.167	0.023	0.00	3.71	-0.95
	0.167	0.668	0.023	3.21	-1.85	-0.95
	0.167	0.168	0.022	0.02	0.01	3.79
	0.334	0.334	0.110	-3.09	-1.78	-1.31
	0.334	0.834	0.109	0.00	3.57	-1.30
	0.834	0.334	0.109	3.09	-1.79	-1.30
	0.834	0.834	0.110	0.00	0.00	3.80
	0.000	0.000	0.197	-3.10	-1.79	-1.27
	1.000	0.500	0.197	0.00	3.58	-1.27
	0.500	0.000	0.197	3.10	-1.79	-1.27
	0.500	0.500	0.197	0.00	0.00	3.80
	0.666	0.666	0.285	-3.09	-1.78	-1.31
	0.666	0.166	0.285	0.00	3.57	-1.30
	0.166	0.666	0.285	3.09	-1.79	-1.30
	0.166	0.166	0.285	0.00	0.00	3.80
	0.332	0.332	0.373	-3.17	-1.83	-1.10
	0.332	0.833	0.372	0.01	3.71	-0.95
	0.833	0.332	0.372	3.21	-1.85	-0.95
	0.833	0.832	0.372	0.02	0.01	3.79
Oxygen Ion	0.001	0.001	0.001	-0.02	-0.01	-0.02
	0.500	0.500	0.001	0.00	0.00	0.02
	0.002	0.501	0.001	0.00	0.02	-0.01
	0.501	0.002	0.001	0.02	-0.01	-0.01
	0.334	0.835	0.045	0.00	0.00	-0.01
	0.835	0.334	0.045	0.00	0.00	-0.01
	0.834	0.834	0.045	0.00	0.00	0.00
	0.334	0.334	0.045	0.00	0.00	-0.01
	0.667	0.667	0.087	0.00	0.00	0.00
	0.167	0.167	0.087	0.00	0.00	0.01
	0.667	0.167	0.087	0.00	0.00	0.00
	0.167	0.667	0.087	0.00	0.00	0.00
	0.000	0.501	0.131	0.00	0.00	0.00
	0.500	0.000	0.131	0.00	0.00	0.00
	0.500	0.500	0.131	0.00	0.00	0.00
	0.000	0.000	0.131	0.00	0.00	0.00
	0.333	0.333	0.175	0.00	0.00	0.00
	0.833	0.833	0.175	0.00	0.00	0.00
	0.333	0.833	0.175	0.00	0.00	0.00
	0.833	0.334	0.175	0.00	0.00	0.00
	0.667	0.167	0.219	0.00	0.00	0.00
	0.167	0.666	0.219	0.00	0.00	0.00
	0.167	0.167	0.219	0.00	0.00	0.00
	0.667	0.667	0.219	0.00	0.00	0.00
	1.000	1.000	0.263	0.00	0.00	0.00
	0.500	0.500	0.263	0.00	0.00	0.00
	1.000	0.499	0.263	0.00	0.00	0.00
	0.500	1.000	0.263	0.00	0.00	0.00
	0.333	0.833	0.308	0.00	0.00	0.00
	0.833	0.333	0.308	0.00	0.00	0.00
	0.833	0.833	0.307	0.00	0.00	0.01
	0.333	0.333	0.308	0.00	0.00	0.00
	0.666	0.666	0.350	0.00	0.00	-0.01
	0.166	0.166	0.350	0.00	0.00	0.00
	0.666	0.165	0.350	0.00	0.00	-0.01
	0.165	0.666	0.350	0.00	0.00	-0.01
	0.998	0.499	0.394	0.00	0.02	-0.01
	0.499	0.998	0.394	0.02	-0.01	-0.01
	0.500	0.500	0.394	0.00	0.00	0.02
	0.999	0.999	0.394	-0.02	-0.01	-0.02

Table 21: The ionic positions and magnetic structure of the PuO_2 $cH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.500	0.500	0.931	0.00	0.00	0.00
	0.501	0.499	0.910	0.00	0.00	0.00
	0.499	0.501	0.485	0.00	0.00	0.00
	0.500	0.500	0.463	0.00	0.00	0.00
Actinide Ion	0.666	0.668	0.022	-3.21	-1.86	-0.93
	0.666	0.167	0.022	0.00	3.71	-0.92
	0.166	0.668	0.022	3.21	-1.86	-0.93
	0.166	0.167	0.022	0.00	0.01	3.79
	0.333	0.334	0.109	-3.09	-1.78	-1.31
	0.333	0.834	0.109	0.00	3.57	-1.30
	0.833	0.334	0.109	3.09	-1.78	-1.31
	0.833	0.834	0.109	0.00	0.00	3.80
	0.000	0.000	0.197	-3.10	-1.79	-1.26
	1.000	0.500	0.197	0.00	3.58	-1.26
	0.500	0.000	0.197	3.10	-1.79	-1.27
	0.500	0.500	0.197	0.00	0.00	3.80
	0.667	0.666	0.285	-3.09	-1.78	-1.31
	0.667	0.166	0.285	0.00	3.57	-1.30
	0.167	0.666	0.285	3.09	-1.78	-1.31
	0.167	0.166	0.285	0.00	0.00	3.80
	0.334	0.332	0.372	-3.21	-1.86	-0.93
	0.334	0.833	0.372	0.00	3.71	-0.93
	0.834	0.332	0.372	3.21	-1.86	-0.93
	0.834	0.833	0.372	0.00	0.01	3.79
Oxygen Ion	0.999	0.001	0.001	-0.02	-0.01	-0.02
	0.499	0.501	0.001	0.00	0.00	0.02
	0.999	0.501	0.001	0.00	0.02	-0.02
	0.499	0.001	0.001	0.02	-0.01	-0.02
	0.333	0.834	0.045	0.00	0.00	-0.01
	0.833	0.334	0.045	0.00	0.00	-0.01
	0.833	0.834	0.045	0.00	0.00	0.00
	0.333	0.334	0.045	0.00	0.00	-0.01
	0.666	0.667	0.087	0.00	0.00	0.00
	0.166	0.167	0.087	0.00	0.00	0.01
	0.666	0.167	0.087	0.00	0.00	0.00
	0.166	0.667	0.087	0.00	0.00	0.00
	1.000	0.501	0.131	0.00	0.00	0.00
	0.500	0.001	0.131	0.00	0.00	0.00
	0.500	0.501	0.131	0.00	0.00	0.00
	0.999	0.000	0.131	0.00	0.00	0.00
	0.333	0.333	0.175	0.00	0.00	0.00
	0.833	0.833	0.175	0.00	0.00	0.00
	0.333	0.834	0.175	0.00	0.00	0.00
	0.833	0.333	0.175	0.00	0.00	0.00
	0.667	0.166	0.219	0.00	0.00	0.00
	0.167	0.667	0.219	0.00	0.00	0.00
	0.167	0.167	0.219	0.00	0.00	0.00
	0.667	0.667	0.219	0.00	0.00	0.00
	0.001	1.000	0.263	0.00	0.00	0.00
	0.500	0.499	0.263	0.00	0.00	0.00
	0.000	0.499	0.263	0.00	0.00	0.00
	0.500	0.999	0.263	0.00	0.00	0.00
	0.334	0.833	0.308	0.00	0.00	0.00
	0.834	0.333	0.308	0.00	0.00	0.00
	0.834	0.833	0.307	0.00	0.00	0.01
	0.334	0.333	0.308	0.00	0.00	0.00
	0.667	0.666	0.350	0.00	0.00	-0.01
	0.167	0.166	0.350	0.00	0.00	0.00
	0.667	0.166	0.350	0.00	0.00	-0.01
	0.167	0.666	0.350	0.00	0.00	-0.01
	0.001	0.499	0.394	0.00	0.02	-0.01
	0.501	0.999	0.394	0.02	-0.01	-0.02
	0.501	0.499	0.394	0.00	0.00	0.02
	0.001	0.999	0.394	-0.02	-0.01	-0.01

Table 22: The ionic positions and magnetic structure of the PuO_2 $dH_{2(111)}$ configurations.

	Ionic Position (Direct)			Magnetic Vector (μ_B)		
	z-Axis	y-Axis	x-Axis	z-Axis	y-Axis	x-Axis
Hydrogen Ion	0.334	0.830	0.937	0.00	0.00	0.00
	0.334	0.833	0.915	0.00	0.00	0.00
	0.666	0.167	0.479	0.00	0.00	0.00
	0.666	0.170	0.458	0.00	0.00	0.00
Actinide Ion	0.667	0.666	0.022	-3.21	-1.85	-0.95
	0.667	0.166	0.022	0.00	3.71	-0.95
	0.167	0.666	0.022	3.21	-1.85	-0.95
	0.167	0.166	0.022	0.00	0.01	3.79
	0.334	0.333	0.109	-3.09	-1.78	-1.31
	0.334	0.833	0.109	0.00	3.57	-1.31
	0.834	0.333	0.109	3.09	-1.78	-1.31
	0.834	0.833	0.109	0.00	0.00	3.80
	0.000	0.000	0.197	-3.10	-1.79	-1.27
	1.000	0.500	0.197	0.00	3.58	-1.27
	0.500	0.000	0.197	3.10	-1.79	-1.27
	0.500	0.500	0.197	0.00	0.00	3.80
	0.666	0.667	0.285	-3.09	-1.78	-1.31
	0.666	0.167	0.285	0.00	3.57	-1.31
	0.166	0.667	0.285	3.09	-1.78	-1.31
	0.166	0.167	0.285	0.00	0.00	3.80
	0.333	0.334	0.372	-3.21	-1.85	-0.95
	0.333	0.834	0.372	0.00	3.71	-0.95
	0.833	0.334	0.372	3.21	-1.85	-0.95
	0.833	0.834	0.372	0.00	0.01	3.79
Oxygen Ion	0.001	0.999	0.001	-0.02	-0.01	-0.01
	0.501	0.499	0.001	0.00	0.00	0.02
	0.001	0.499	0.001	0.00	0.02	-0.02
	0.501	0.999	0.001	0.02	-0.01	-0.01
	0.334	0.833	0.045	0.00	0.00	-0.01
	0.835	0.332	0.045	0.00	0.00	-0.01
	0.834	0.833	0.044	0.00	0.00	0.00
	0.334	0.332	0.045	0.00	0.00	-0.01
	0.667	0.666	0.087	0.00	0.00	0.00
	0.167	0.166	0.087	0.00	0.00	0.01
	0.667	0.166	0.087	0.00	0.00	0.00
	0.167	0.666	0.087	0.00	0.00	0.00
	0.000	0.500	0.131	0.00	0.00	0.00
	0.501	0.999	0.131	0.00	0.00	0.00
	0.500	0.499	0.131	0.00	0.00	0.00
	0.000	0.999	0.131	0.00	0.00	0.00
	0.333	0.333	0.175	0.00	0.00	0.00
	0.833	0.833	0.175	0.00	0.00	0.00
	0.333	0.833	0.175	0.00	0.00	0.00
	0.834	0.333	0.175	0.00	0.00	0.00
	0.667	0.167	0.219	0.00	0.00	0.00
	0.166	0.667	0.219	0.00	0.00	0.00
	0.167	0.167	0.219	0.00	0.00	0.00
	0.667	0.667	0.219	0.00	0.00	0.00
	1.000	0.001	0.263	0.00	0.00	0.00
	0.500	0.501	0.263	0.00	0.00	0.00
	1.000	0.500	0.263	0.00	0.00	0.00
	0.499	0.001	0.263	0.00	0.00	0.00
	0.333	0.834	0.308	0.00	0.00	0.00
	0.833	0.334	0.308	0.00	0.00	0.00
	0.833	0.834	0.307	0.00	0.00	0.01
	0.333	0.334	0.308	0.00	0.00	0.00
	0.666	0.668	0.350	0.00	0.00	-0.01
	0.166	0.167	0.350	0.00	0.00	0.00
	0.666	0.167	0.350	0.00	0.00	-0.01
	0.165	0.668	0.350	0.00	0.00	-0.01
	0.999	0.501	0.394	0.00	0.02	-0.01
	0.499	0.001	0.394	0.02	-0.01	-0.01
	0.499	0.501	0.393	0.00	0.00	0.02
	0.999	0.001	0.394	-0.02	-0.01	-0.01

2.4 Bader Charges

A Bader charge analysis with the Henkleman *et al*[2-4] code has been completed.[5] The inequivalent actinide (An(a)-An(d)) and oxygen (O(e)-O(l)) ions for each surface are labelled (**Figure 3**). Note: as an inherent issue common to DFT-based methods, the Bader charges of the ions are often underestimated.[6]

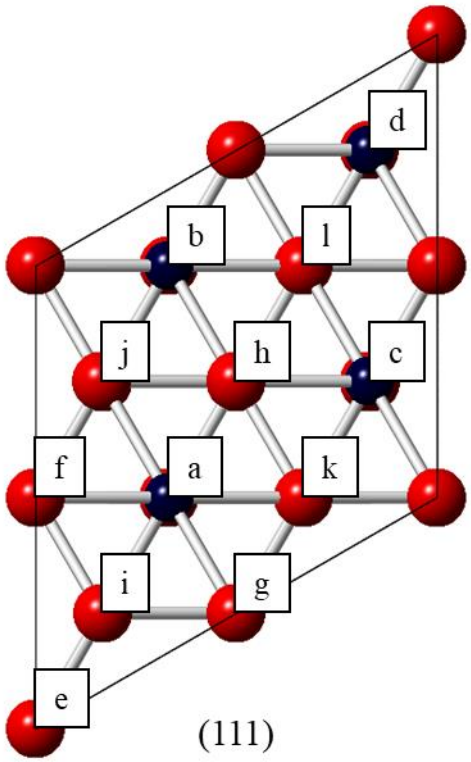

Figure 3: The inequivalent actinide (An_a-An_d) and oxygen (O_e-O_l) ions for the low-index AnO_2 (111) surface are indicated (surface 3 monolayers).

Table 23: The Bader charge distribution (eV) of the UO_2 (111) surface for each configuration.

Configuration	H		U				O							
	α	β	a	b	c	d	e	f	g	h	i	j	k	l
Clean Surface														
	-	-	2.55	2.55	2.56	2.55	-1.28	-1.28	-1.28	-1.27	-1.30	-1.30	-1.30	-1.30
Atomic Interaction														
a	-0.35	-	2.67	2.58	2.59	2.58	-1.29	-1.28	-1.28	-1.28	-1.23	-1.23	-1.23	-1.27
b	0.61	-	2.54	2.54	2.54	2.19	-1.29	-1.25	-1.29	-1.29	-1.28	-1.33	-1.28	-1.28
Molecular Interaction														
a	0.00	0.01	2.55	2.55	2.55	2.55	-1.30	-1.30	-1.30	-1.29	-1.27	-1.28	-1.27	-1.28
b	0.00	0.00	2.55	2.56	2.55	2.55	-1.30	-1.30	-1.30	-1.30	-1.27	-1.28	-1.27	-1.28
c	0.00	0.00	2.55	2.56	2.56	2.55	-1.30	-1.30	-1.30	-1.30	-1.27	-1.27	-1.27	-1.27
d	0.00	0.00	2.56	2.55	2.56	2.56	-1.30	-1.30	-1.30	-1.30	-1.28	-1.27	-1.28	-1.28
e	-0.01	0.00	2.56	2.55	2.56	2.55	-1.30	-1.30	-1.30	-1.30	-1.27	-1.28	-1.27	-1.28

Table 24: The Bader charge distribution (eV) of the NpO_2 (111) surface for each configuration.

Configuration	H		Np				O							
	α	β	a	b	c	d	e	f	g	h	i	j	k	l
Clean Surface														
	-	-	2.51	2.51	2.51	2.51	-1.25	-1.25	-1.25	-1.25	-1.24	-1.25	-1.25	-1.25
Atomic Interaction														
a	0.57	-	2.48	2.10	2.48	2.48	-1.27	-1.27	-1.25	-1.27	-1.26	-1.26	-1.28	-1.26
Molecular Interaction														
a	0.02	-0.01	2.52	2.52	2.51	2.51	-1.25	-1.25	-1.24	-1.25	-1.25	-1.25	-1.25	-1.25
b	-0.04	0.04	2.25	2.53	2.48	2.48	-1.25	-1.25	-1.24	-1.25	-1.25	-1.25	-1.25	-1.25
c	0.03	-0.03	2.51	2.53	2.51	2.51	-1.25	-1.25	-1.24	-1.25	-1.25	-1.25	-1.25	-1.25
d	-0.04	0.04	2.51	2.52	2.49	2.49	-1.24	-1.25	-1.24	-1.25	-1.25	-1.25	-1.25	-1.25
e	0.01	-0.01	2.51	2.53	2.50	2.50	-1.25	-1.25	-1.24	-1.25	-1.25	-1.25	-1.25	-1.25

Table 25: The Bader charge distribution (eV) of the PuO_2 (111) surface for each configuration.

Configuration	H		Pu				O							
	α	β	a	b	c	d	e	f	g	h	i	j	k	l
Clean Surface														
	-	-	2.45	2.44	2.44	2.47	-1.24	-1.24	-1.24	-1.22	-1.21	-1.23	-1.23	-1.23
Atomic Interaction														
a	-0.03	-	2.41	2.45	2.45	2.47	-1.22	-1.21	-1.23	-1.22	-1.22	-1.22	-1.21	-1.23
b	0.58	-	2.45	2.45	2.45	2.08	-1.26	-1.22	-1.26	-1.26	-1.25	-1.25	-1.28	-1.24
Molecular Interaction														
a	0.02	-0.01	2.44	2.45	2.45	2.46	-1.22	-1.21	-1.23	-1.23	-1.24	-1.24	-1.23	-1.24
b	0.02	-0.01	2.44	2.45	2.45	2.47	-1.22	-1.21	-1.23	-1.23	-1.24	-1.24	-1.23	-1.24
c	-0.05	0.05	2.45	2.45	2.45	2.47	-1.22	-1.21	-1.22	-1.23	-1.24	-1.23	-1.23	-1.23
d	0.06	-0.06	2.45	2.45	2.45	2.47	-1.22	-1.21	-1.23	-1.22	-1.24	-1.24	-1.23	-1.24

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