Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Magnetic Structure of UO_2 and NpO_2 by First-Principle Methods (Additional Information)

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Keywords: Nuclear Fuel, Uranium Dioxide, Neptunium Dioxide, Noncollinear, Magnetism, DFT, Small-Moment. Multi-k states, Transverse, Longitudinal.

The final relaxed ionic structures (calculated by HSE06 with SOI included) are shown (Table A1-A19).

Table A1: The final relaxed UO_2 structure for the DM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.44802	0.00000	0.00000
	0.00000	5.44802	0.00000
	0.00000	0.00000	5.44802
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A2: The final relaxed UO_2 structure for the FM (001) configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45532	0.00000	0.00000
	0.00000	5.45532	0.00000
	0.00000	0.00000	5.46953
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A3: The final relaxed UO_2 structure for the FM (011) configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45672	0.00000	0.00000
	0.00000	5.46242	0.00000
	0.00000	0.00000	5.46242
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.24908	0.25000	0.25000
	0.25092	0.25000	0.75000
	0.25092	0.75000	0.25000
	0.24908	0.75000	0.75000
	0.75092	0.75000	0.75000
	0.74908	0.75000	0.25000
	0.74908	0.25000	0.75000
	0.75092	0.25000	0.25000

Table A4: The final relaxed UO_2 structure for the FM (111) configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45815	-0.00625	-0.00625
	-0.00625	5.45815	-0.00625
	-0.00625	-0.00625	5.45815
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.24986	0.24986	0.24986
	0.25014	0.25014	0.75014
	0.25014	0.75014	0.25014
	0.24986	0.74986	0.74986
	0.75014	0.75014	0.75014
	0.74986	0.74986	0.24986
	0.74986	0.24986	0.74986
	0.75014	0.25014	0.25014

Table A5: The final relaxed UO_2 structure for the longitudinal 1k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45653	0.00000	0.00000
	0.00000	5.45653	0.00000
	0.00000	0.00000	5.46208
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A6: The final relaxed UO_2 structure for the longitudinal 2k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45567	0.00000	0.00000
	0.00000	5.45734	0.00000
	0.00000	0.00000	5.45734
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A7: The final relaxed UO_2 structure for the longitudinal 3k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45660	0.00000	0.00000
	0.00000	5.45660	0.00000
	0.00000	0.00000	5.45660
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A8: The final relaxed UO_2 structure for the transverse 1k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45519	0.00000	0.00000
	0.00000	5.45305	0.00000
	0.00000	0.00000	5.46382
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A9: The final relaxed UO_2 structure for the transverse 2k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45529	0.00000	0.00000
	0.00000	5.45310	0.00000
	0.00000	0.00000	5.46415
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.24998	0.25000
	0.25000	0.25002	0.75000
	0.25000	0.74998	0.25000
	0.25000	0.75002	0.75000
	0.75000	0.75002	0.75000
	0.75000	0.74998	0.25000
	0.75000	0.25002	0.75000
	0.75000	0.24998	0.25000

Table A10: The final relaxed UO_2 structure for the transverse 3k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.45775	0.00000	0.00000
	0.00000	5.45775	0.00000
	0.00000	0.00000	5.45775
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.24636	0.24636	0.24636
	0.24636	0.25364	0.74636
	0.25364	0.74636	0.24636
	0.25364	0.75364	0.74636
	0.75364	0.75364	0.75364
	0.75364	0.74636	0.25364
	0.74636	0.25364	0.75364
	0.74636	0.24636	0.25364

Table A11: The final relaxed NpO_2 structure for the FM (001) configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.41431	0.00000	0.00000
	0.00000	5.41431	0.00000
	0.00000	0.00000	5.41490
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A12: The final relaxed NpO_2 structure for the FM (011) configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.41590	0.00000	0.00000
	0.00000	5.41580	-0.03616
	0.00000	-0.03616	5.41580
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.24924	0.25000	0.25000
	0.25076	0.25000	0.75000
	0.25076	0.75000	0.25000
	0.24924	0.75000	0.75000
	0.75076	0.75000	0.75000
	0.74924	0.75000	0.25000
	0.74924	0.25000	0.75000
	0.75076	0.25000	0.25000

Table A13: The final relaxed NpO_2 structure for the FM (111) configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.41550	-0.02032	-0.02032
	-0.02032	5.41550	-0.02032
	-0.02032	-0.02032	5.41550
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.24953	0.24953	0.24953
	0.25047	0.25047	0.75047
	0.25047	0.75047	0.25047
	0.24953	0.74953	0.74953
	0.75047	0.75047	0.75047
	0.74953	0.74953	0.24953
	0.74953	0.24953	0.74953
	0.75047	0.25047	0.25047

Table A14: The final relaxed NpO_2 structure for the longitudinal 1k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.41609	0.00000	0.00000
	0.00000	5.41609	0.00000
	0.00000	0.00000	5.41271
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A15: The final relaxed NpO_2 structure for the longitudinal 2k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.41212	0.00000	0.00000
	0.00000	5.41493	0.00000
	0.00000	0.00000	5.41493
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A16: The final relaxed NpO_2 structure for the longitudinal 3k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.41397	0.00000	0.00000
	0.00000	5.41397	0.00000
	0.00000	0.00000	5.41397
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A17: The final relaxed NpO_2 structure for the transverse 1k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.40535	0.00000	0.00000
	0.00000	5.42420	0.00000
	0.00000	0.00000	5.41410
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.25000	0.25000	0.25000
	0.25000	0.25000	0.75000
	0.25000	0.75000	0.25000
	0.25000	0.75000	0.75000
	0.75000	0.75000	0.75000
	0.75000	0.75000	0.25000
	0.75000	0.25000	0.75000
	0.75000	0.25000	0.25000

Table A18: The final relaxed NpO_2 structure for the transverse 2k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.41609	0.00000	0.00000
	0.00000	5.41479	0.00000
	0.00000	0.00000	5.41459
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.24767	0.24766	0.24766
	0.24767	0.25234	0.74766
	0.25233	0.74766	0.24766
	0.25233	0.75234	0.74766
	0.75233	0.75234	0.75234
	0.75233	0.74766	0.25234
	0.74767	0.25234	0.75234
	0.74767	0.24766	0.25234

Table A19: The final relaxed NpO_2 structure for the transverse 3k AFM configuration (calculated by HSE06). The dimensions of the unit cell are given in the angstroms (Å); whereas, the ionic positions are given in terms of fractional coordinates.

	Coordinates		
	X	Y	Z
Unit Cell	5.41423	0.00000	0.00000
	0.00000	5.41423	0.00000
	0.00000	0.00000	5.41423
Ionic Positions	0.00000	0.00000	0.00000
	0.50000	0.50000	0.00000
	0.50000	0.00000	0.50000
	0.00000	0.50000	0.50000
	0.24770	0.24770	0.24770
	0.24770	0.25230	0.74770
	0.25230	0.74770	0.24770
	0.25230	0.75230	0.74770
	0.75230	0.75230	0.75230
	0.75230	0.74770	0.25230
	0.74770	0.25230	0.75230
	0.74770	0.24770	0.25230