

**Supporting Information:**

**Topology of the Electron Density and of its  
Laplacian from Periodic LCAO Calculations on  
*f*-Electron Materials: The Case of Cesium  
Uranyl Chloride**

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# 1 Crystal Input for $\text{Cs}_2\text{UO}_2\text{Cl}_4$

CS2U02Cl4

CRYSTAL

0 0 0

12

11.78820 7.64110 5.76860 100.4380

4

292 0.00000 0.00000 0.00000

255 0.66487 0.00000 0.32067

17 0.39809 0.24695 0.20704

8 0.11906 0.00000 0.23790

END

292 31

INPUT

32. 0 4 8 8 8 6

16.91870874 529.53526911 0

3.40970576 4.27018845 0

0.79302733 0.09998874 0

0.19378381 0.00626781 0

13.16953414 100.93359134 0

10.60784728 175.95423897 0

2.69049397 -0.00210787 0

2.08929800 -0.19041648 0

0.54050990 0.00494627 0

0.40482776 -0.01652483 0

0.11250285 0.00082033 0

0.09508873 -0.00100028 0

9.06784123 62.85927902 0

8.53362678 90.20882494 0  
 1.63646790 -0.08282418 0  
 1.54425719 -0.15307917 0  
 0.47961552 -0.00008720 0  
 0.41164502 0.00484078 0  
 0.13990510 -0.00006136 0  
 0.17494682 -0.00240839 0  
 5.14746012 15.68628229 0  
 5.29241394 22.32105345 0  
 1.05726701 -0.20689333 0  
 0.98063114 -0.08434451 0  
 0.48259555 0.06084446 0  
 0.55434882 0.00231264 0  
 0.23674544 -0.00204069 0  
 0.21559852 0.00348388 0  
 18.83643086 -44.41029420 0  
 18.74850924 -53.65339478 0  
 6.49279545 -2.55219343 0  
 6.57472519 -3.34380088 0  
 2.58151924 0.04527524 0  
 2.58690949 0.05637947 0  
 0 0 1 2 1  
 29520.834 1.  
 0 0 1 2 1  
 4449.8874 1.  
 0 0 1 2. 1  
 1018.7754 1.  
 0 0 1 0 1  
 289.5348 1.

0 0 1 0 1  
46.9990 1.  
0 0 1 0 1  
23.9791 1.  
0 0 1 0 1  
10.1441 1.  
0 0 1 0 1  
2.7658 1.  
0 0 1 0 1  
0.6151 1.  
0 0 1 0 1  
0.2780 1.  
0 2 1 6 1  
499.7488 1.  
0 2 1 6 1  
114.0192 1.  
0 2 1 0 1  
15.6492 1.  
0 2 1 0 1  
7.9843 1.  
0 2 1 0 1  
3.1325 1.  
0 2 1 0 1  
1.6077 1.  
0 2 1 0 1  
0.7061 1.  
0 2 1 0 1  
0.3229 1.  
0 3 1 10 1

75.1703 1.  
 0 3 1 1 1  
 20.7869 1.  
 0 3 1 0 1  
 5.5167 1.  
 0 3 1 0 1  
 2.6058 1.  
 0 3 1 0 1  
 1.2781 1.  
 0 3 1 0 1  
 0.5617 1.  
 0 3 1 0 1  
 0.2135 1.  
 0 4 1 3. 1  
 8.1761 1.  
 0 4 1 0 1  
 3.5111 1.  
 0 4 1 0 1  
 1.6789 1.  
 0 4 1 0 1  
 0.7604 1.  
 0 4 1 0 1  
 0.3170 1.  
 0 5 1 0 1  
 0.7604 1  
 255 3  
 HAYWSC  
 0 1 3 8 1  
 2.7869668567 0.0406474598702 -0.0165526980724

1.15910578043 -0.555331349468 -0.156354595401

0.444885148239 0.790078910046 0.653388515688

0 1 1 1 1

0.152606321165 1. 1.

0 3 1 0 1

0.599990264849 1.

17 13

0 0 7 2 1

69507.9909450	0.54314897497D-03
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10426.1568800	0.41990463961D-02
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2373.2334061	0.21592141679D-01
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671.56420071	0.84598850094D-01
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218.41999790	0.24757249724
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77.572249714	0.47016930228
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28.888815277	0.37436370716
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0 0 3 2 1

127.10527185	0.25182166603D-01
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39.339582961	0.10786112456
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7.6740679989	-0.27408821574
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0 0 2 2 1

3.8745627630	1.3213875014
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1.8385832573	0.68636955368
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0 0 1 0 1

0.50229057542	1.0000000
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0 0 1 0 1

0.17962723420	1.0000000
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0 2 5 6 1

666.50423284	0.23632663836D-02
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157.64241690	0.18879300374D-01
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50.262520978	0.87206341273D-01
18.536078105	0.25285612970
7.2940532777	0.43507154820
0 2 1 5 1	
2.9433248995	.35026513165
0 2 1 0 1	
1.0404970818	1.0000000
0 2 1 0 1	
0.38456415080	1.0000000
0 2 1 0 1	
0.13069642732	1.0000000
0 3 2 0 1	
4.61000000	0.20000000
1.01100000	1.00000000
0 3 1 0 1	
0.339000000	1.0000000
0 4 1 0 1	
0.706000000	1.0000000
8 11	
0 0 6 2 1	
27032.3826310	0.21726302465D-03
4052.3871392	0.16838662199D-02
922.32722710	0.87395616265D-02
261.24070989	0.35239968808D-01
85.354641351	0.11153519115
31.035035245	0.25588953961
0 0 2 2 1	
12.260860728	0.39768730901
4.9987076005	0.24627849430

0 0 1 0 1		
	1.1703108158	1.0000000
0 0 1 0 1		
	0.46474740994	1.0000000
0 0 1 0 1		
	0.18504536357	1.0000000
0 2 4 4 1		
	63.274954801	0.60685103418D-02
	14.627049379	0.41912575824D-01
	4.4501223456	0.16153841088
	1.5275799647	0.35706951311
0 2 1 0 1		
	0.52935117943	.44794207502
0 2 1 0 1		
	0.17478421270	.24446069663
0 3 1 0 1		
	2.31400000	1.0000000
0 3 1 0 1		
	0.64500000	1.0000000
0 4 1 0 1		
	1.42800000	1.0000000
99 0		
END		
DFT		
XXLGRID		
B3LYP		
ENDDFT		
TOLINTEG		
8 8 8 8 20		



MAXCYCLE

200

FMIXING

95

SMEAR

0.0001

SHRINK

6 6

TOLDEE

9

PPAN

END