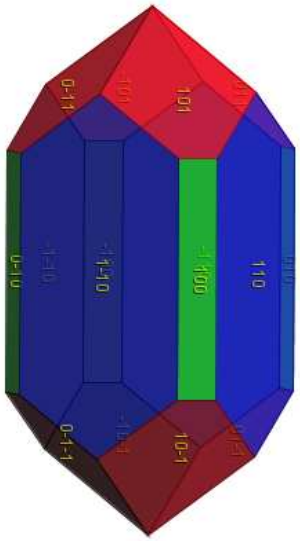
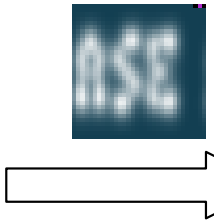
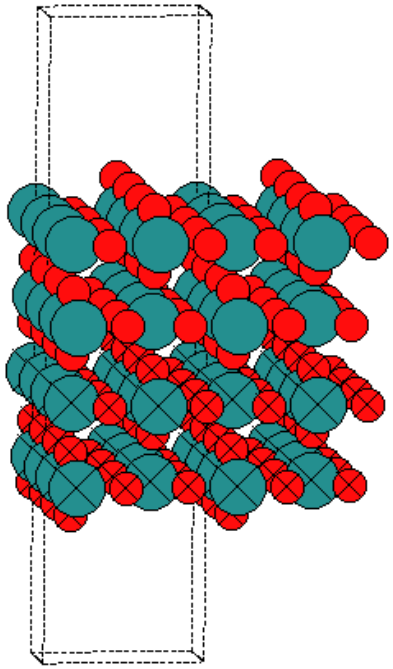
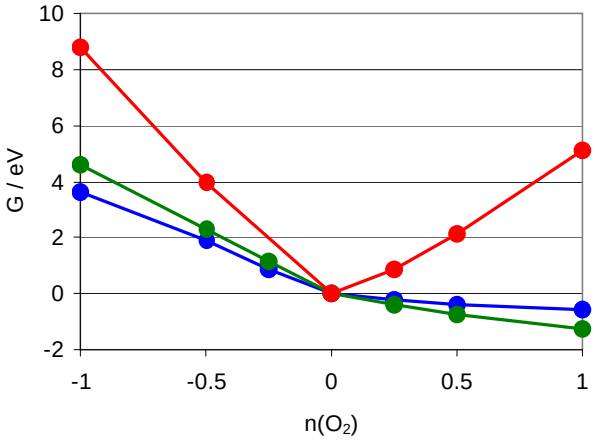






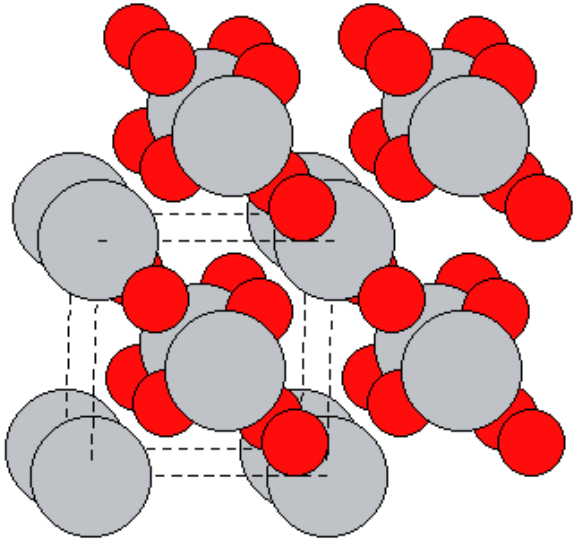


My first experiences with ASE, GPAW and surface calculations.

Ansgar Schäfer

SUNCAT @ SLAC, Aug. – Oct. 2010

Lattice constants of rutile structures



TiO_2 rutile: a = b = 4.59 A, c = 2.96 A (exp.*)
tetragonal crystal system
spacegroup 136 (P42/mnm)

Fully optimized MO_2 rutile structures:

	experiment *		RPBE		PBE		LDA	
	a / A	c / A	a / A	c / A	a / A	c / A	a / A	c / A
Ti	4.592	2.957	4.687	2.977	4.651	2.962	4.555	2.918
Ir	4.498	3.154	4.631	3.225				
Ru	4.492	3.107	4.654	3.186				
Cr	4.421	2.917	4.626	2.748				
Pb	4.957	3.387	5.222	3.468				

* American Mineralogist Crystal Structure Database
(rruff.geo.arizona.edu/AMS)

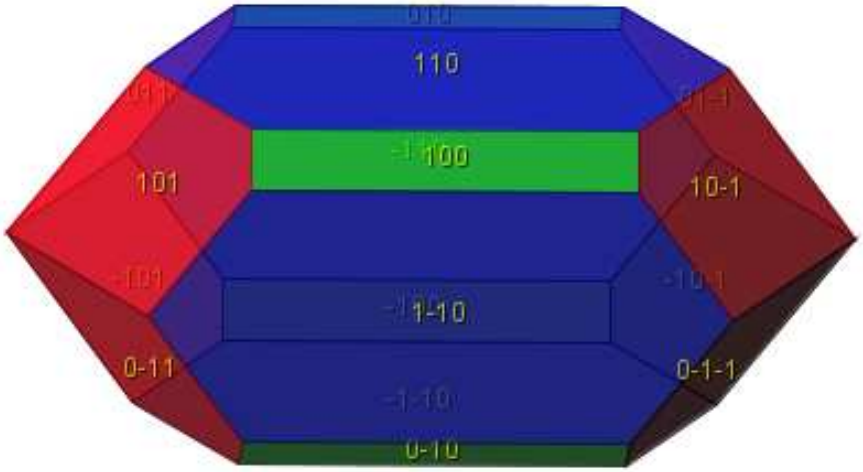
TiO2 structure optimization using the „rmm-diis“ eigensolver

Mixer			structure #1		structure #2		structure #3	
beta	nmaxold	weight	#iter	last E	#iter	last E	#iter	last E
0.05	3	10	>120	-49.69904				
0.05	3	50	69	-49.69904	>120	-49.71204		
0.05	3	250	62	-49.69874	>120	-49.71202		
0.05	5	10	>120	-49.69894				
0.05	5	50	42	-49.69913	>120	-49.71203		
0.05	5	250	34	-49.69937	31	-49.71196	0	-49.72620
0.05	7	10	>120	-49.69889				
0.05	7	50	69	-49.69856	>120	-49.71203		
0.05	7	250	>120	-49.69903				
0.1	3	10	33	-49.69899	>120	-49.71205		
0.1	**3**	**50**	**35**	**-49.69906**	**>120**	**-49.71203**		
0.1	3	250	35	-49.69906	>120	-49.71204		
0.1	5	10	>120	-49.69818				
0.1	5	50	>120	-49.69813				
0.1	5	250	>120	-49.69811				
0.1	7	10	39	-49.69971	>120	-49.71204		
0.1	7	50	36	-49.69929	>120	-49.71204		
0.1	7	250	>120	-49.69904				
0.2	3	10	31	-49.69893	>120	-49.71204		
0.2	3	50	>120	-49.69904				
0.2	3	250	31	-49.69904	>120	-49.71204		
0.2	5	10	93	-49.69904	>120	-49.71204		
0.2	5	50	31	-49.69870	>120	-49.71204		
0.2	5	250	31	-49.69860	>120	-49.71204		
0.2	7	10	41	-49.69914	>120	-49.71204		
0.2	7	50	34	-49.69937	62	-49.71204	0	-49.72620
0.2	7	250	>120	-49.69904				
0.25	3	1	>120	-49.69904				
0.25	7	1000	>120	-49.69904				
0.05	5	1000	37	-49.69919	>120	-49.71206		

TiO2 structure optimization using the „cg“ eigensolver

Mixer			structure #1		structure #2		structure #3		structure #4		
beta	nmaxold	weight	#iter	last E	#iter	last E	#iter	last E	#iter	last E	∑ iter
0.05	3	10	29	-49.69910	15	-49.71202	22	-49.72611	12	-49.72644	78
0.05	3	50	33	-49.69951	14	-49.71216	18	-49.72664	15	-49.72663	80
0.05	3	250	36	-49.69860	14	-49.71206	19	-49.72637	15	-49.72664	84
0.05	5	10	44	-49.69889	13	-49.71200	16	-49.72613	13	-49.72653	86
0.05	5	50	38	-49.69914	13	-49.71210	16	-49.72617	12	-49.72666	79
0.05	5	250	37	-49.69921	13	-49.71199	16	-49.72572	13	-49.72664	79
0.05	7	10	28	-49.69909	13	-49.71208	16	-49.72632	13	-49.72657	70
0.05	7	50	36	-49.69940	14	-49.71189	16	-49.72627	14	-49.72681	80
0.05	7	250	38	-49.69893	13	-49.71217	16	-49.72636	13	-49.72690	80
0.1	3	10	24	-49.69914	13	-49.71195	14	-49.72612	12	-49.72670	63
0.1	**3**	**50**	**24**	**-49.69899**	**14**	**-49.71198**	**14**	**-49.72635**	**12**	**-49.72696**	**64**
0.1	3	250	23	-49.69915	14	-49.71180	14	-49.72625	12	-49.72669	63
0.1	5	10	25	-49.69899	13	-49.71224	13	-49.72627	11	-49.72683	62
0.1	5	50	30	-49.69867	13	-49.71226	13	-49.72626	11	-49.72683	67
0.1	5	250	27	-49.69909	13	-49.71232	13	-49.72629	11	-49.72680	64
0.1	7	10	24	-49.69916	12	-49.71205	14	-49.72618	11	-49.72639	61
0.1	7	50	23	-49.69895	12	-49.71203	14	-49.72606	11	-49.72635	60
0.1	7	250	23	-49.69918	12	-49.71206	14	-49.72612	11	-49.72636	60
0.2	3	10	20	-49.69922	10	-49.71180	14	-49.72612	9	-49.72669	53
0.2	3	50	20	-49.69908	10	-49.71179	14	-49.72610	9	-49.72669	53
0.2	3	250	19	-49.69910	10	-49.71181	14	-49.72616	9	-49.72668	52
0.2	5	10	20	-49.69949	11	-49.71212	13	-49.72616	9	-49.72657	53
0.2	5	50	19	-49.69895	11	-49.71211	13	-49.72615	9	-49.72656	52
0.2	5	250	18	-49.69892	11	-49.71211	13	-49.72613	9	-49.72658	51
0.2	7	10	19	-49.69923	11	-49.71216	13	-49.72639	9	-49.72656	52
0.2	7	50	19	-49.69909	11	-49.71217	13	-49.72639	9	-49.72657	52
0.2	7	250	19	-49.69901	11	-49.71215	13	-49.72639	9	-49.72657	52
0.2	3	4	20	-49.69925	10	-49.71199	13	-49.72615	9	-49.72669	52
0.2	3	2	20	-49.69928	10	-49.71199	14	-49.72620	9	-49.72669	53
0.2	3	1	20	-49.69924	10	-49.71199	13	-49.72619	9	-49.72670	52
0.3	3	50	17	-49.69949	11	-49.71214	12	-49.72631	10	-49.72647	50
0.4	3	50	16	-49.69904	12	-49.71200	13	-49.72603	10	-49.72643	51
0.5	3	50	18	-49.69912	12	-49.71206	14	-49.72608	11	-49.72655	55

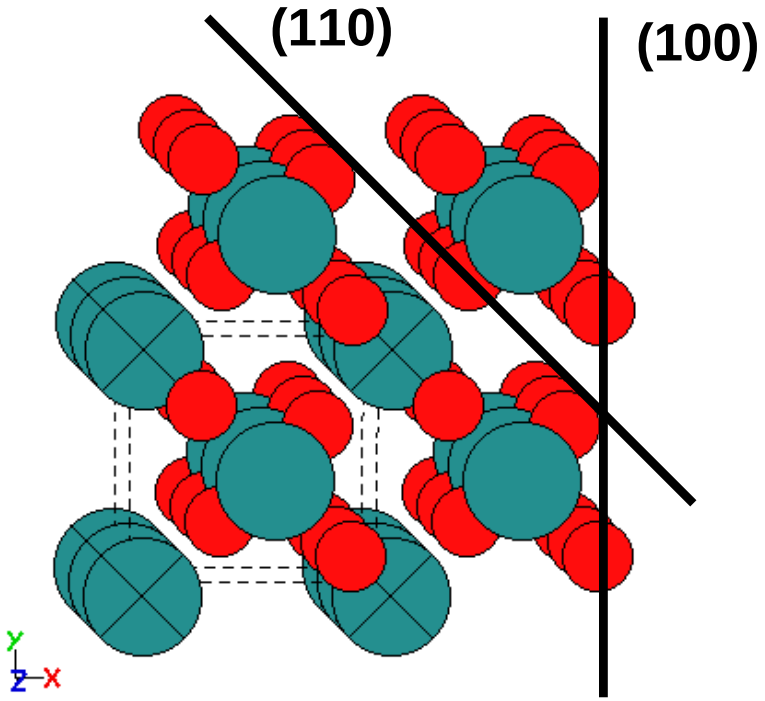
Rutile crystal surfaces

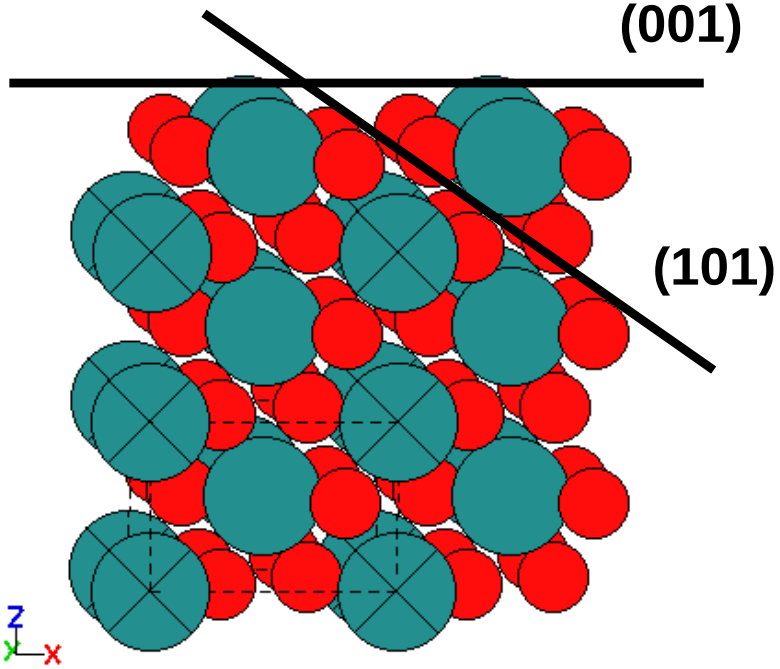


(110)

(101)

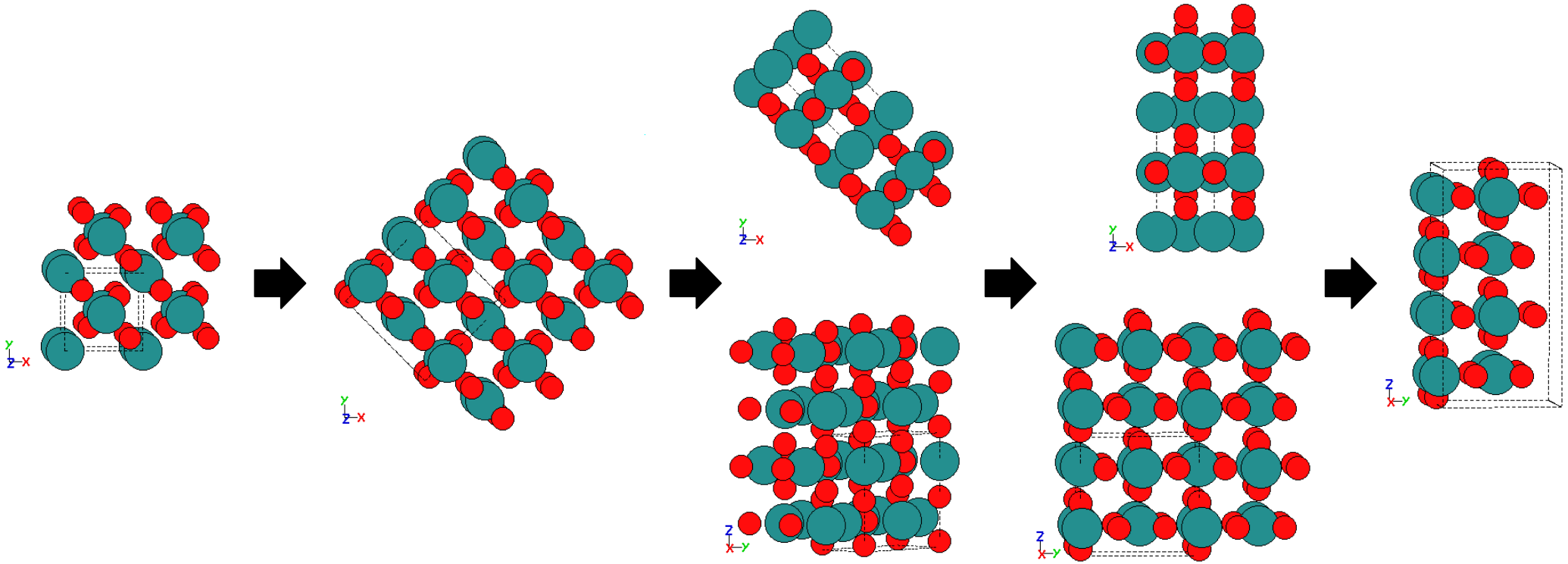
(100)



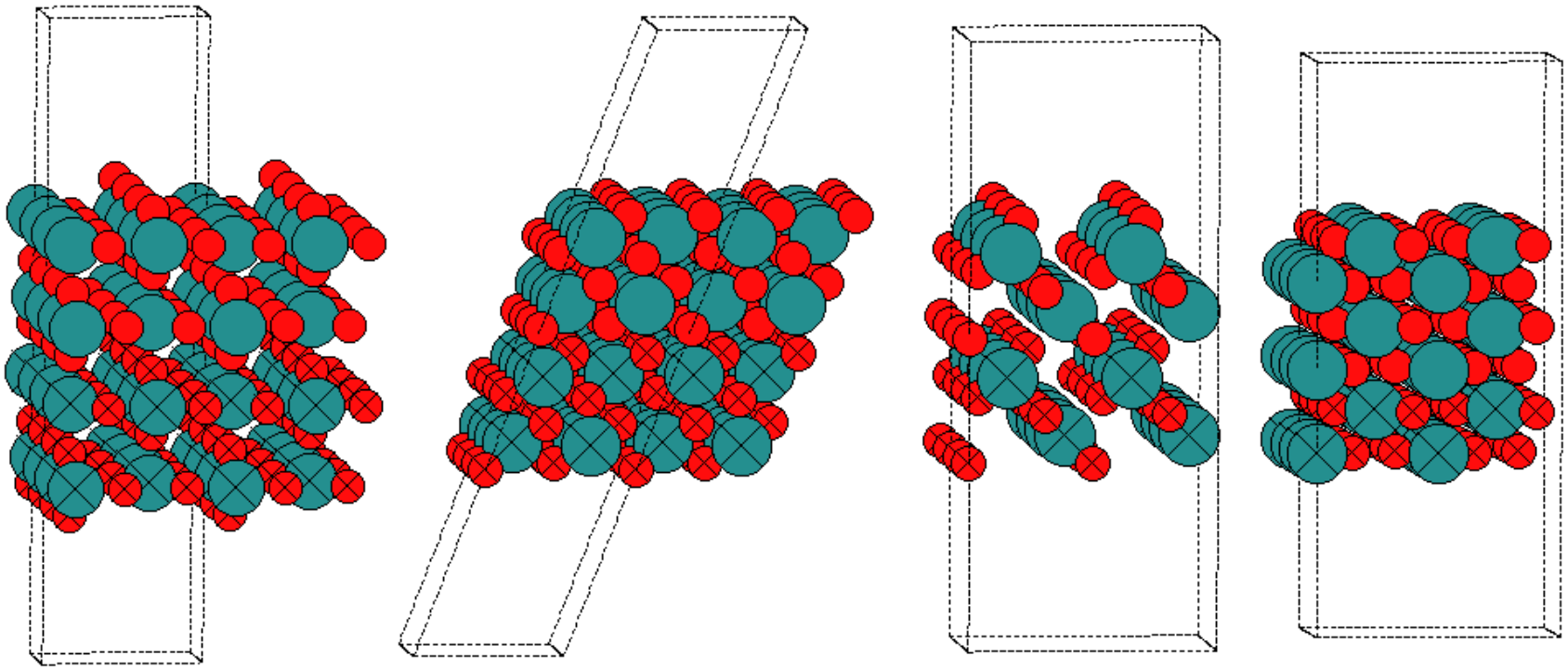


Generating surfaces with the ASE tools

```
from ase.utils.geometry import cut
bulk_110 = cut(bulk, a=(0,0,1), b=(1,-1,0), c=(1,1,0), origo=(.25,.25,0))
bulk_110.rotate((1,1,0), (0,0,1), center=(0,0,0), rotate_cell=True)
bulk_110.rotate('z', pi*3/4, center=(0,0,0), rotate_cell=True)
slab_110 = bulk_110.repeat((2,1,2))
slab_110.center(vacuum=7.0, axis=2)
```



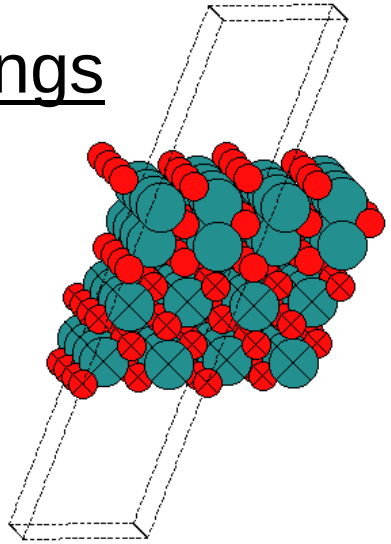
Stoichiometric RuO2 surface structures and energies



ΔE (eV / A^2) relative to bulk

	(110)	(101)	(100)	(001)
relaxed	0.056	0.063	0.067	0.087
unrelaxed	0.069	0.084	0.090	0.120

Performance test of GPAW parameter settings



RuO_2 (101) 1x2x2 with O-defects: $Ru_{16}O_{28}$

Unit cell: a = 5.64 A, b = 9.31 A, c = 25.20 A (ca. 14 A vacuum)

alpha = gamma = 90°, beta = 68.80°

Computer: 4x8 X5550@2.67GHz

		mixer		poisson solver		convergence		energy	wall time	
eigensolver	nbands	beta / nmaxold / weight	grid	relax / eps	fermi	eigenstates / density	# iter.	eV	s	
cg	n(AOs)	0.10 / 5 / 10	28, 52, 132	J / 1e-10	0.10	1e-8 / 1e-4	43	-291.48205	12886	+/- 100
dav							51	-291.48251	5049	
rmm-diis							49	-291.48194	2657	
rmm-diis	-30						55	-291.48272	2132	
rmm-diis	-25						55	-291.48280	2101	
rmm-diis	-20						59	-291.48276	2065	
rmm-diis	-15						89	-291.48277	2885	
rmm-diis	-10						>120			
rmm-diis	-5						>120			
cg	-15						54	-291.48286	9934	
rmm-diis	-15	0.10 / 5 / 50					91	-291.48262	2939	
rmm-diis	-15	0.10 / 3 / 10					96	-291.48299	3412	
rmm-diis	-15	0.10 / 7 / 10					88	-291.48272	13238	
rmm-diis	-15	0.20 / 5 / 10					>120			
rmm-diis	-15	0.05 / 5 / 10					80	-291.48275	2594	
rmm-diis			32,56,136				53	-290.91614	21683	
rmm-diis			32,48,136				54	-291.16848	17143	
rmm-diis				J / 1e-7			89	-291.48405	25296	
rmm-diis				GS / 1e-10			43	-291.48267	21767	
rmm-diis	-20	0.05 / 5 / 10					54	-291.48203	1852	
rmm-diis	-20				0.20		73	-291.57051	2550	
rmm-diis	-20				0.05		59	-291.44056	2198	
rmm-diis	-20				0.02		58	-291.41651	2111	
rmm-diis	-20	0.05 / 5 / 10				1e-7 / 1e-4	53	-291.48193	1912	