

K Point size and optimizer	a /Å	b/Å	c/Å	c/a	Equatorial / Å	Axial / Å	Total Energy /eV	Band Gap /eV
4 4 8 LBFGS Free	4.633	4.634	2.997	2.997/4.633 = 0.6469	2.00 2.00	1.94 1.94 1.94	-425.5990	3.12
4 4 8 LBFGS Angles fixed to 90 degrees	4.607	4.607	2.998	2.998/4.633 = 0.6471	2.00 2.00	1.94 1.94	-425.5713	3.11
4 4 8 Fix angles LBFGS Angles fixed to 90 degrees Force tolerance 1E-6	4.632	4.635	2.997	0.6466	2.00 1.99 2.00	1.92 2.00	-425.5990	3.12
4 4 8 Conjugate Gradient	4.672	4.672	2.997	2.997/4.672 = 0.6415	1.99 1.99	1.99 1.99 1.99	-425.6037	3.13
4 4 8 Conjugate Gradient Constraint used: Isotropic	4.643	4.643	2.995	2.995/4.643 = 0.6451	1.99 2.00	2.00 1.93 1.93	-425.5972	3.11
4 4 8 CG Angles fixed to 90 degrees	4.180	4.180	4.176	0.999	3.46 3.46	1.81 1.81 1.81	-425.4453	3.928

4 4 8 gDIIS	4.6 72	4.6 72	2.9 97	2.997/4 .672 = 0.6415	1.99 2.00	1.9 3 2.0 0 1.9 2	-425.603 7	3.13
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