

	$a$ (Å)	$c$ (Å)	$u$	$c/a$	$v_0$ (Å <sup>3</sup> )
LDA	4.552	2.922	0.3038	0.642	60.55
r <sup>2</sup> SCAN	4.602	2.961	0.3046	0.643	62.71
PBESOL	4.595	2.942	0.3044	0.640	62.12

# References

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- [2] J. R. DeVore, *Journal of Applied Physics*, **96**, 4112 (2004).