

Supplementary Information: Exploring Correlation Effects and Volume Collapse During 1D-0D Electride Subspace Reduction in Ca_2N

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Table 1: Lattice parameters for Ca₂N taken from Ref.¹

Symmetry group	Lattice parameter (Å)	Atom	Wykoff position	x	y	z
$Fd\bar{3}m$	a = 9.69	Ca	32e	0.6155	0.3845	0.6155
		N	16d	0.1250	0.1250	0.6250
$I\bar{4}2d$	a = 7.12	Ca	16e	0.3114	0.5658	0.6806
	c = 7.23	N	8d	0.7500	0.1314	0.8750

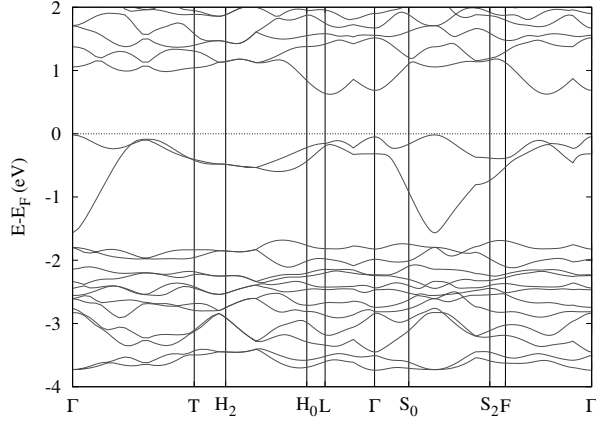


Figure 1: Band structure of $I\bar{4}2d$ phase of Ca₂N.

References

- (1) Tang, H.; Wan, B.; Gao, B.; Muraba, Y.; Qin, Q.; Yan, B.; Chen, P.; Hu, Q.; Zhang, D.; Wu, L. et al. Metal-to-Semiconductor Transition and Electronic Dimensionality Reduction of Ca₂N Electride under Pressure. *Advanced Science* **2018**, *5*, 2–7.