

SILICON HEXABORIDE INVESTIGATIONS USING *ab initio* DATA MINING APPROACH



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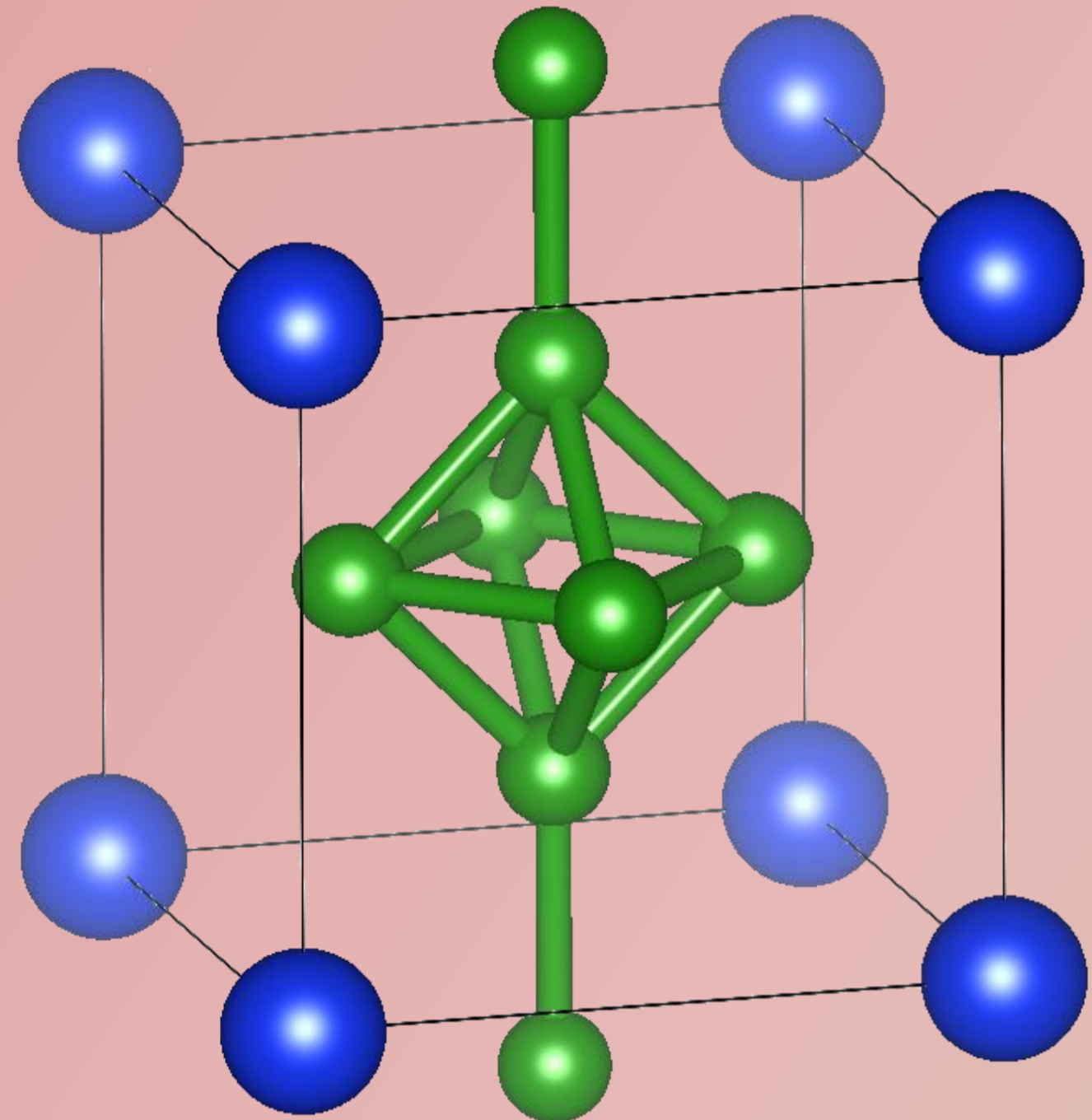
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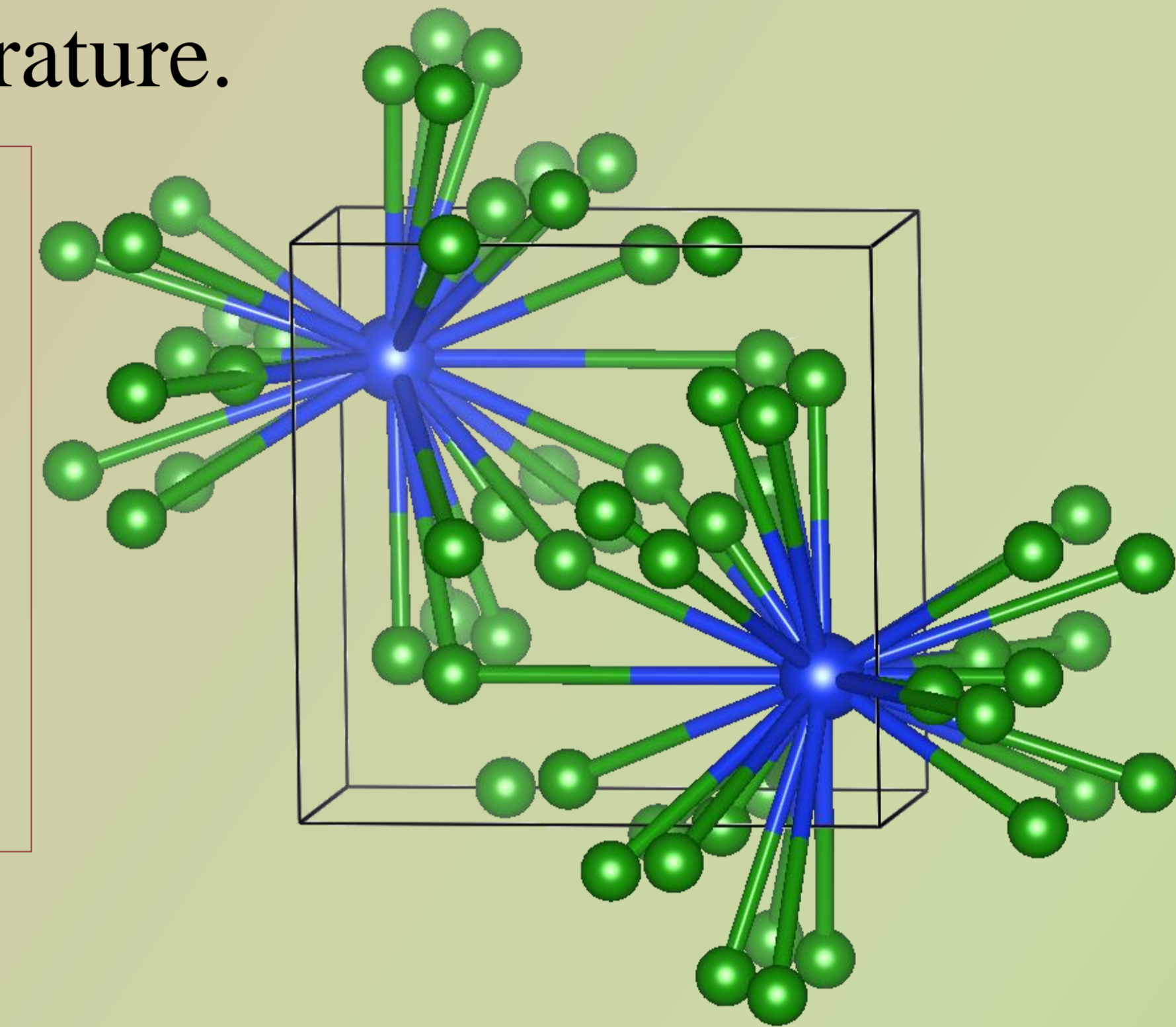
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Silicon borides are light weight ceramics with very wide application due to their outstanding properties. Silicon hexaboride is a very desirable industrial material discovered in 1900 and it is considered to be one of the most enigmatic refractory compound. On the other hand, the crystal structure is yet not fully understood in the literature.

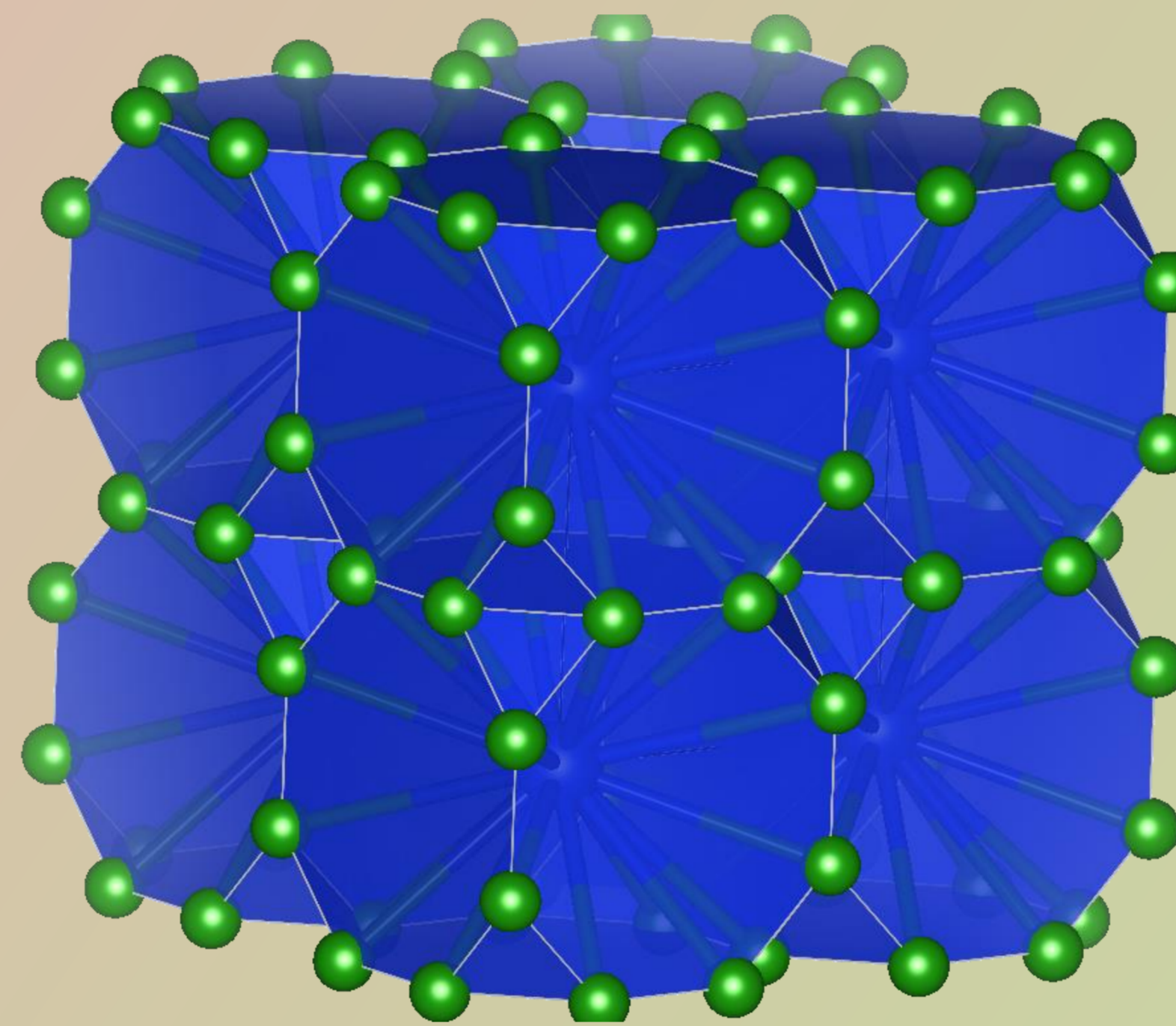
The first reports suggested a cubic SiB₆, which was followed by experimentally observed orthorhombic phase. Later studies, determined a cubic SiB₆ as an unstable phase and suggested additional monoclinic P21/m space group.



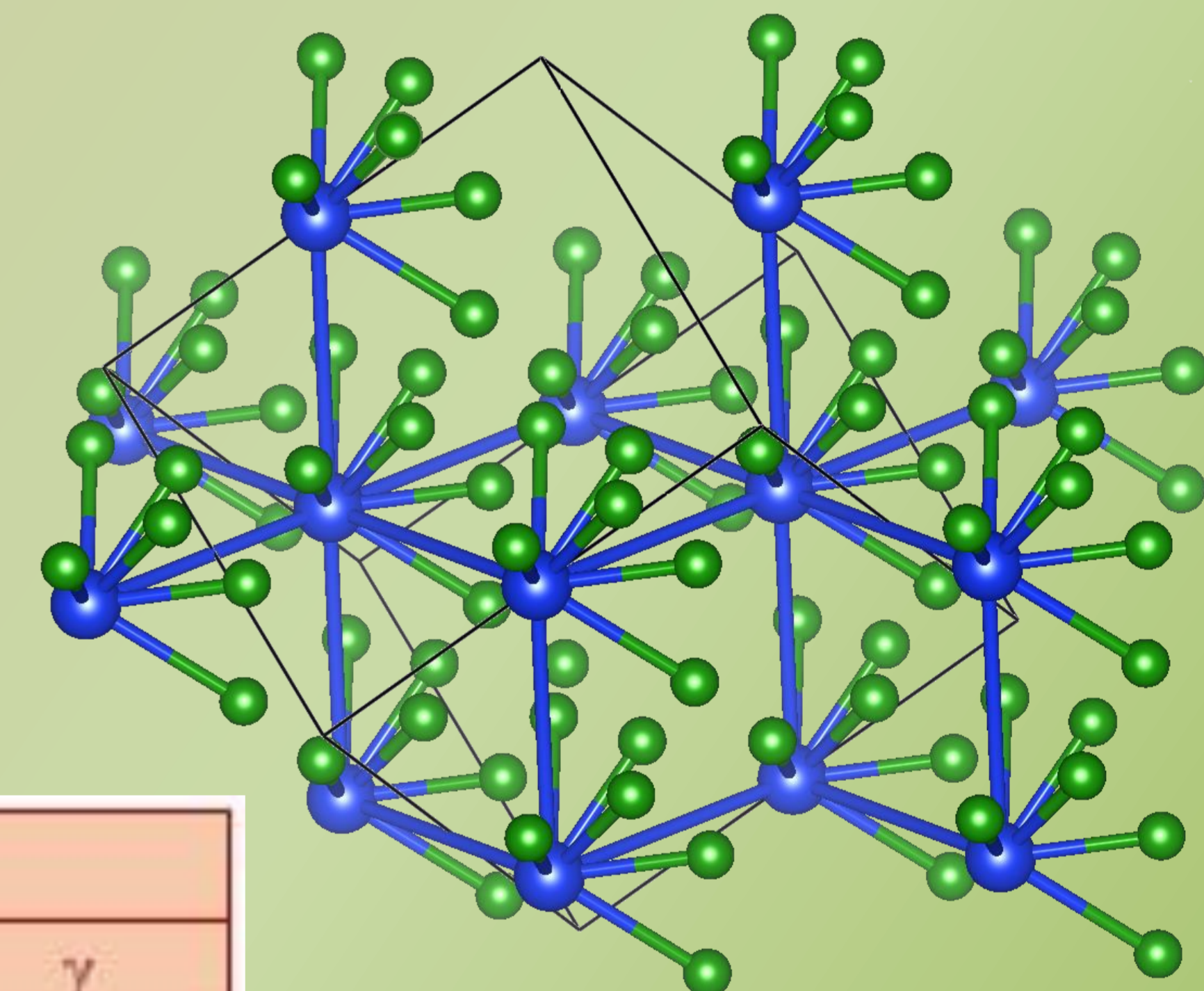
Pm-3m
SiB₆ cubic – B-B atoms



P21/m
SiB₆ – monoclinic



Pm-3m
SiB₆ cubic – Si-B atoms



R 3 m
SiB₆ - rhombohedral



Pm-3m
SiB₆ cubic – Si-Si atoms

Space group and modification	Cell parameters					
	a	b	c	α	β	γ
<i>Pm-3m</i> (221)	4.13000	4.13000	4.13000	90.0000	90.0000	90.0000
<i>P21/m</i> (11)	6.26000	6.22000	3.07000	90.0000	90.0300	90.0000
<i>R 3 m</i> (160)	5.85000	5.85000	7.48000	90.0000	90.0000	120.0000

Goal is investigation of suggested phase and prediction of novel structure candidates within this system. Since the ability to operate in the extreme environments of SiB₆ modifications was considered, it is very important to future explore these newly discovered phases and investigate in detail their properties in order to find new possibilities for future industrial and technological applications.

Methods

We have undertaken calculations using *ab initio* minimization data mining. Unknown structure candidates found in the SiB₆ system have been generated using data mining, followed by local optimization. *Ab Initio* calculations were carried out on density functional theory (DFT) level using LDA and GGA functional.

Elastic constants and mechanical properties for each of the predicted modification have been investigated.

References

- [1] D. Zagorac, J. C. Schön, M. Jansen, *Processing and Application of Ceramics* **7** (2013) 37.
 [2] J. Zagorac, D. Zagorac, A. Zarubica, J. C. Schön, K. Djuris, B. Matovic, *Acta Crystallographica Section B* **70** (2014) 809.