The Fifth Element in the Periodic Table, Boron: Do we know the Ground State Structure?

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Boron exhibits the most complex structure of all elemental solids, with more than 300 atoms per unit cell arranged in interconnecting icosahedra. The best estimate on the number of atoms in the unit-cell is not even an integer number, 320.1, originating from the introduction of partial occupancy of atomic sites in the X-ray structural analysis [1].

This work is the first attempt, using *ab initio* molecular dynamics, to study the stable configuration of the partially occupied sites (POS) in β-boron and to investigate POS impact on the electronic structure. We have found that the correlated POS configurations not only lower the total energy of the solid, but also widen the electronic band gap, giving consistent results with experiments.

The high pressure phases of boron[2,3] have also been studied with *ab initio* simulated annealing methods. We found that at around 120GPa, β-rhombohedral boron undergoes amorphization and that its electronic conductivity rises, due to delocalization of the electronics states near the Fermi level, consistent with experimental observations[2,3].

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