

**Dipole moment of quasi-planar boron clusters.** / R. Becker, L. Chkhartishvili. / Nano Studies. – 2015. – # 11. – pp. 29-48. – eng.

Boron crystallizes in complex structures containing several non-equivalent atomic sites with different coordination numbers. Shifting of the electron density towards to the highly-coordinated atoms yields the palpable polarization of all-boron lattices, in general unexpected in elemental crystals. Same effect has to be inherent of boron clusters as well. We have experimental evidences that boron vapor consists of small clusters  $B_n$ , which are known to exhibit (quasi)planar structures (for number of boron atoms  $n$  not more than about 15). For all ground-state isomers of them we have estimated effective atomic charges and for asymmetric species – dipole moment as well. Binding energies per atom of (quasi)planar boron clusters, theoretically determined from the B–B interatomic pair potential, have been refined taking into account the obtained polarity of a part of B–B bonds. Fig. 2, Tab. 1, Ref. 88.

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