Abstract Submitted
for the TSS13 Meeting of
The American Physical Society

Electronic structure of planar aggregates of boron clusters CARLOS DIAZ, LUIS BASURTO, TUNNA BARUAH, RAJENDRA ZOPE, UTEP — Using simulated annealing, random searches and basin hopping, we have searched for low lying isomers of boron cluster containing 27 atoms in its neutral and charged states. For those searches, the interatomic potential between boron atoms is described using density functional theory at the generalized gradient approximation level. The structures of low lying isomers found in our searches are predominantly quasi-planar. Several of these structures are seen as growth of smaller size boron clusters. The population of low energy neutral boron cluster isomers was used to study the influence that charge has on the structural pattern of charged boron clusters. The calculations indicate that the boron clusters also tend to prefer quasi-planar geometries. These are the largest planar boron cluster aggregates reported so far. Electronic properties such as ionization energies, vertical detachment energies and electron affinities and also the infrared and Raman spectra of neutral clusters will be presented.

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Date submitted: 01 Mar 2013 Electronic form version 1.4