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A new family of chiral boron fullerenes and related planar boron sheet RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — Using the recent idea of balancing two-center and three-center bondings between boron atoms, a new class of stable chiral boron nanostructures (fullerenes and nanotubes) is designed. The structures of these fullerenes consist of triangular and hexagonal motifs similar to those seen in the most stable α-boron sheet and the B_{80} fullerene. The binding energy of the new sheet is only 0.02 eV lower than that of the α-boron sheet. Our density functional calculations show that these new boron nanostructures are energetically competitive with the recently proposed α-boron nanostructures. For example, B_{60}, the smallest member of this new $60n^2$ boron fullerene family, is 0.7 eV more stable than exact boron equivalent of icosahedral C_{60} fullerene.

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