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Boron a frustrated element: ab-initio study of pressure induced amorphization¹ TADASHI OGITSU, FRANCOIS GYGI, GIULIA GALLI, Lawrence Livermore National Laboratory — At ambient conditions, boron exhibits the most complex structure of all elemental solids, with an intricate arrangement of interconnecting icosahedra and more than 300 atoms per unit cell. It is the only element purified in significant quantities whose ground state structure has not been fully determined. We have performed ab-initio study of boron at ambient condition and under pressure. At low P and temperature, our results favor a quasi-ordered, crystalline ground state with an even number of atoms per unit cell (320) and a finite density of states at the Fermi level. Due to the highly localized nature of these states, boron turns out to be non conductive, in agreement with experiment. At about 100 GPa, we observe an order-to-disorder transition, which occurs by a series of hierarchical structural changes. Contrary to intuition based on bond strength arguments, the “short,” inter-icosahedral bonds are broken first, followed by a partial rupture of icosahedral units with “longer” bonds, eventually leading to full disruption of long range order, consistent with recent measurements. Above 120 GPa, we find a notable increase in electronic conductivity, due to delocalization of electronic states, yielding a poor metallic state.

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