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Theoretical studies on structural and electronic properties of boron and boron nitride nanodiscs: A density functional approach

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Using first principles density functional theory calculations, we systematically studied the structural and electronic properties of boron nano disc (B-nd) and boron nitride nano disc(BN- nd). By using state of art method we designed two novel structures of B-nd and BN-nd with average diameter of 0.8578 nm and 0.7487 nm respectively. These structures are optimized using sufficient conjugate gradient steps followed by individual convergence test of Mesh-cutoff, K- points and lattice constants. After structural optimization our *ab-initio* calculation calculated cohesive energy per pair of atoms to verify the stability of structures in generalized gradient approximation (GGA) within the SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) package. The main feature of SIESTA is the use of flexible basis sets composed of linear combination of numerical atomic orbitals, which can be generated by solving the Kohn–Sham equation of atomic pseudopotentials. In order to explore details of electronic properties of these nanodiscs, further density of states, partial/projected density of states, band structure and charge densities of are performed at ambient conditions. These studies show thatBN-nd is comparatively more stable and exhibits semiconducting nature with ~0.6 eV energy gap, whereas B-nd depicting metallic behavior with finite density of states at Fermi energy level. It is found that while doping nitrogen in boron disc it creates energy gap and decreases the conductance also. That mean studied systems may serve as semiconductor as well as metal depending upon the necessity. In the field of materials probably we are first time reporting a novel and theoretical studies on any nanodisc.

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