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Tunable Band Gap of Boron Nitride Interfaces under Uniaxial Pressure[1] ELIZANE MORAES, TAISE MANHABOSCO, ALAN DE OLIVEIRA, RONALDO BATISTA, Federal University of Ouro Preto — In this work we show, by means of a density functional theory formalism, that the interaction between hydrogen terminated boron nitride surfaces gives rise to a metallic interface with free carries of opposite sign at each surface. A band gap can be induced by decreasing the surface separation. The size of the band gap changes continuously from zero up to 4.4 eV with decreasing separation, which is understood in terms of the interaction between surface states.Due to the high thermal conductivity of cubic boron nitride and the coupling between band gap and applied pressure, such tunable band gap interfaces may be used in high stable electronic and electromechanical devices. In addition, the spacial separation of charge carries at the interface may lead to photovoltaic applications.

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