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Origin of Charge Separation in III-Nitride Nanowires under Strain YELONG WU, GUANGDE CHEN, MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China, SU-HUAI WEI, MOWAFAK AL-JASSIM, National Renewable Energy Laboratory, Golden, CO 80401, USA, YANFA YAN, Department of Physics and Astronomy, The University of Toledo, Toledo, OH 43606, USA — The structural and electronic properties of BN, AlN and GaN nanowires (NWs) under different strain condition are investigated using first-principles calculations. We found an anomaly of band gap change with respect to the applied external uniaxial strain. We show that this is due to the band crossing caused by the crystal field splitting at the top of the valence band. Due to the difference of the atomic relaxation at the core and surface regions of the NW, we show that electron and hole separation can be achieved when the compressive uniaxial strain exceeds the critical value $|\epsilon_c|$.

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