Design of Ultraviolet Light Emitting Diodes Based on Hexagonal Boron Nitride

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Ultraviolet light emitting diodes (UV-LEDs) have numerous applications [1] as light sources for disinfection and sterilization, chemical excitation, replacement of UV lamps, etc. Intrinsic large bandgap of hexagonal boron nitride (*h*-BN)[2-3] and the great development in experimental fabrication facilitates the possibility of flexible UV-LEDs. In this work, we perform a series of atomistic simulations to study the core components of *h*-BN-based LED. The multiple quantum wells (MQWs) are created by selectively putting *h*-BN with different stacking orders and thickness together. Quantum confinement for both valence and conduction bands is found. By analyzing the Schottky barrier of contacts between *h*-BN and various metals, promising metal candidates are identified for p- and n-doped h-BN[4-5]. We also calculate the doping effect of *h*-BN under varied doping levels. A concrete LED structure based on *h*-BN is proposed, which gives clear guidance to experimentalists.

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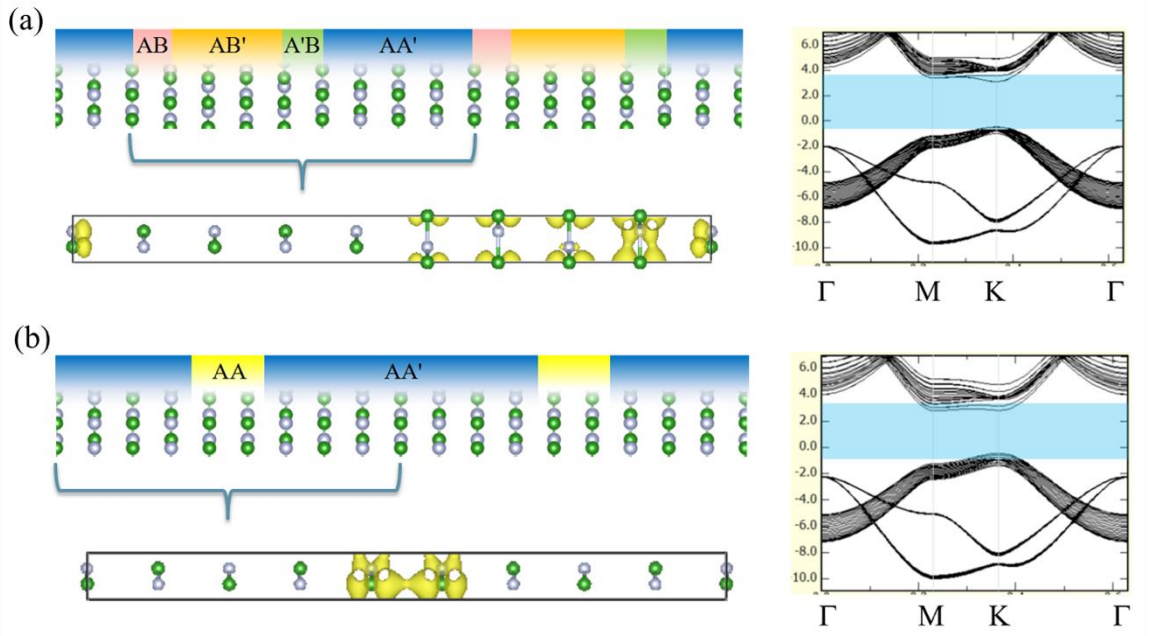

Fig.1: Atomic structures, partial charge densities, and band structures of the two typical multiple quantum wells: (a) MQW-T1 and (b) MQW-T2.

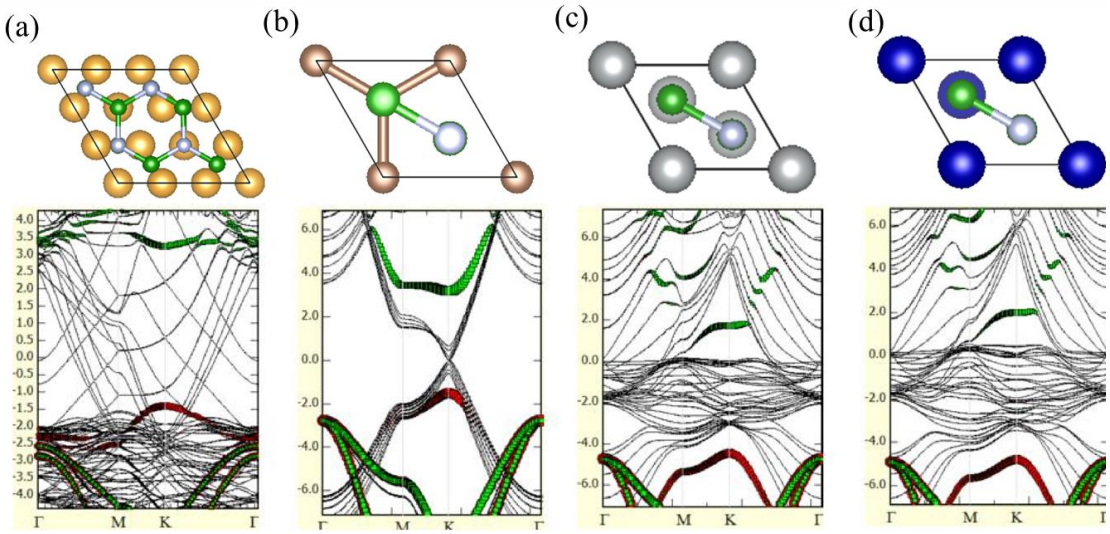

Fig.2: Band structures of monolayer h-BN on (a) Au(111), (b) graphite (0001), (c) Ni(111), and (d) Co(0001).