

## Supporting Information

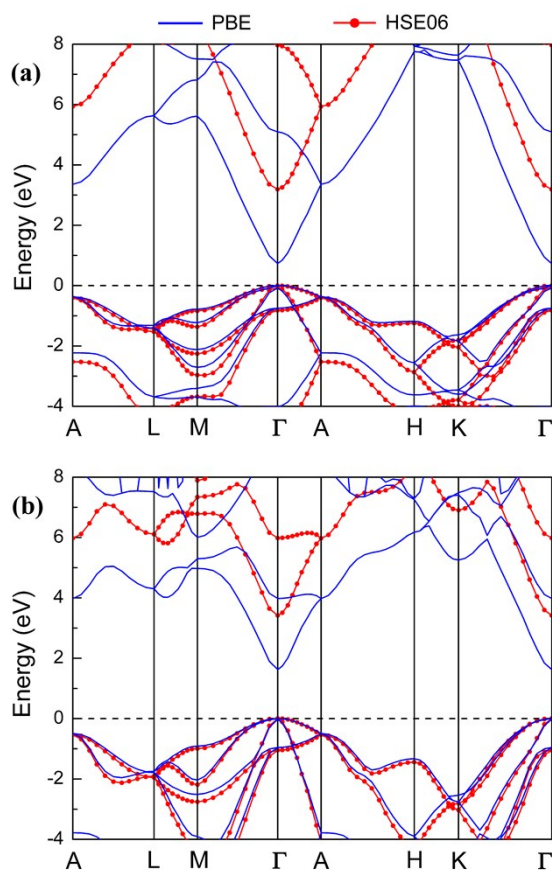
### **Structural and electronic properties of ZnO/GaN heterostructured nanowires from first-principles study**

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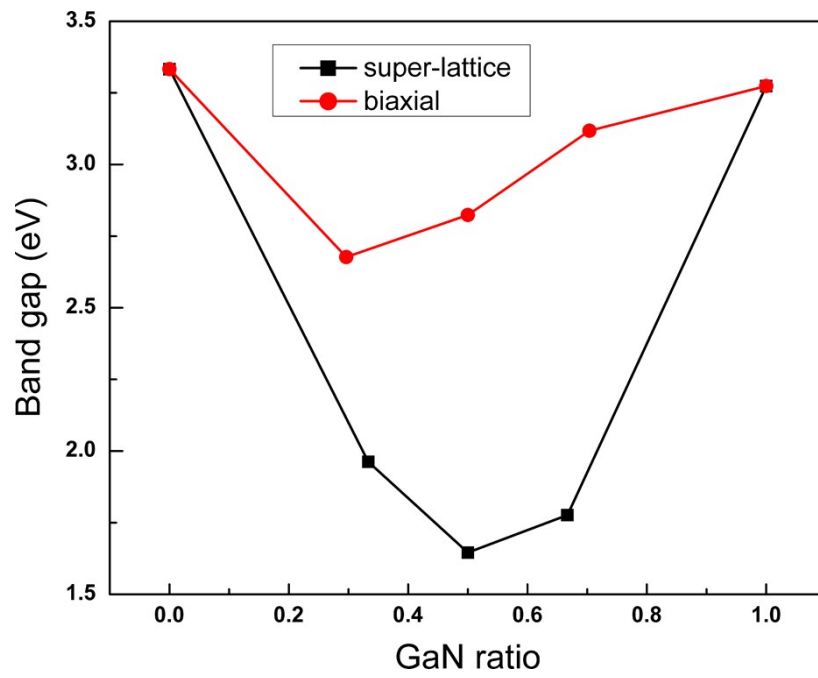
#### Supporting figures:



**Figure S1.** Electronic band structures of wurtzite (a) ZnO and (b) GaN bulks. The band structures denoted by blue solid and red solid-dot lines are calculated by using PBE functional and HSE06. The energy of highest occupied level is set to zero and denoted by the dash line.

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**Figure S2.** Band gaps calculated by HSE06 method as a function of GaN ratio for biaxial and super-lattice heterostructured nanowires with a diameter of 1.65 nm. The GaN ratios of 0.0 and 1.0 respectively represent the pure ZnO and GaN nanowires.