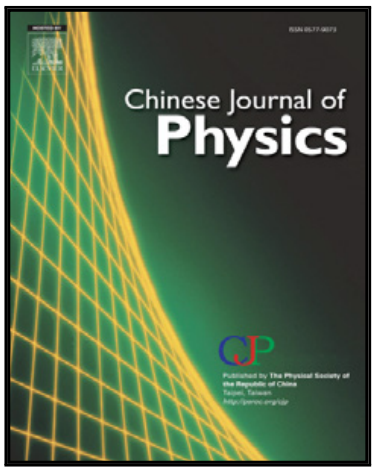

First principles investigation of the structural and electronic properties of (110), (110) and (111) growth axis AlN/GaN superlattices

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Highlights

- We have calculated the electronic properties of AlN and GaN zinc-blende/zinc-blende superlattices (SLs).
- We have calculated the band structures of the (001), (110) and (111) growth axis SLs with *n* varying between 1 and 3.
- The most important results are that all these systems exhibit either a direct or indirect bandgap.
- The partial density of states for the three directions are calculated.
- A larger influence of *sp* and *pd* coupling between the Ga and N atoms explains the nature of the gaps.