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First-principles study of electric field effect on GaN bi- and trilayers DONGWEI XU, HAIYING HE, RAVINDRA PANDEY, Michigan Technological University, SHASHI P. KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: RDRL-WM — First-principles calculations based on density functional theory (DFT) are performed to study bilayers and trilayers of GaN. The calculated results suggest that the bi- and trilayer systems both prefer planar graphene-like configurations rather than buckled bulk-like configurations in their ground states. The most stable configurations are predicted to be the so-called AA$'$ stacking for the bilayer and the AA$'$A stacking for the trilayer at the GGA-DFT level of theory. By appling an external perpendicular electric field to the AB-stacked bilayer, its band gap increases monotonically. However, this is not case for the symmetric AA$'$ stacked bilayer, ABA or AA$'$A stacked trilayer where the applied electric field reduces the band gap. Furthermore, a semiconductor-metal transition is predicted for the ABA stacked GaN trilayer at about 0.4 V/ Å.

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