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The electrostatic and structural properties of GaN nanorods/nanowires from first-principles[1] M.-H. TSAI, Z.-F. JHANG, J.-Y. JIANG, Y.-H. TANG, L.W. TU, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan — The first-principles calculation has revealed that the GaN nanorod has a greatly enhanced dipole moment per area relative to that of a film, which in conjunction with the geometry effect suggests that the top surface of the GaN nanorod has a greater electrostatic attraction for gas-phase Ga and N source species than the film surface during epitaxial growth of GaN, so that nanorods grow much faster than the film. This electrostatic effect may explain the growth of nanorods protruding high above the film surface. The first-principles molecular-dynamics calculation shows that the average Ga-N bond length of the GaN nanowire decreases with the decrease of the diameter of the nanowire, which demonstrates a surface tension effect. This trend can be expected to be the same for the experimentally grown nanorods, because the physical origin that drives this contraction, namely the surface tension, is the same. Thus, the bond-length result may explain the experimentally observed blue shift of the cathodoluminescence emission.

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M.-H. Tsai
Department of Physics, National Sun Yat-Sen University,
Kaohsiung 80424, Taiwan

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