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Reconstructions of the GaN(10$\bar{1}\bar{1}$) surfaces: Density functional theory calculations[1] JUNG-MIN HYUN, Sookmyung Women's University, YONG-SUNG KIM, Korea Research Institute of Standards and Science, HANCHUL KIM, Sookmyung Women's University — GaN has been extensively studied for its potential applicability in optoelectronics as well as in spintronics. The functional performance in such applications depends on the surface characteristics of thin films. Thin films of GaN are typically grown along the polar [0001] direction, but their light-emission efficiency is reduced due to the electron-hole separation. A strategy to remedy such an undesired effect is to grow films along nonpolar or semipolar directions. In this presentation, we will address the reconstructions of the Ga-terminated semipolar (10$\bar{1}\bar{1}$) surface. We performed the density functional theory calculations using the generalized gradient approximation, the projector augmented wave potentials, and the repeated slabs. From the calculated energetics of various reconstructions, we found that there exist a few structural motifs of GaN(10$\bar{1}\bar{1}$). They are short Ga chains and Ga vacancies. For instance, a 4×2 reconstruction with a Ga tetramer and surface Ga vacancies is stable in the N-rich condition, which is significantly different from the previous results [Akiyama *et al*, Jpn. J. Appl. Phys. 48, 100201 (2009)]. Our results would provide a comprehensive understanding on the Ga-terminated semipolar surfaces.

X Prefer Oral Session
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