Theoretical Electron-Energy Loss Study of the electronic structure and optical properties of GaN(0001) and H/GaN(0001)

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GaN surfaces have gained much attention due to the recent technological advances in the nitrides-based optoelectronic devices. The device characteristics depend on the controlled growth nechanisms of GaN thin films, which is essentially a surface process. Therefore, a comprehensive knowledge of the surfaces properties such as atomic structure, electronic and optical properties are highly desirable in these systems.

In this work, we study the electronic and optical properties of the bare and hydrogenated GaN(0001) surfaces, using a First-Principles formalism [1]. This formalism is based in the Density Functional Theory (DFT) within the Local Density Approximation (LDA), and employes the Harris functional, the Hamann-Schlüter-Chiang pseudopotentials [2] and a minimal sp^3 space-localized basis using atomic-like orbitals. For our study, we performe calculations using the generalized self-consistent correction to the Harris LDA functional code called "Fireball96" [3]. Also, we have included excitonic effects to calculate the electronic and optical properties of these surfaces.

For different atomic models of bare and hydrogenated GaN(0001) [4], we calculate their electronic band structure and optical properties for each surface. We analyze in detail the electronic structure and the main optical signature of each surface. The origin of the optical spectra is discussed in terms of the main surface electronic states and of the specific surface atomic rearrangement.

To compare with experimental measurements, we calculate the Electron-Energy Loss Spectra (EELS) for each surface. Results are presented in terms of the dielectric function and EELS, and are compared with recent experimental measurements. Finally, we compare our theoretical results for each surface based in an atomic model with the experimental results. This comparison allows us to explore which atomic reconstruction can be closer to reality.

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