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The fundamental surface science of wurtzite gallium nitride [☆]

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ABSTRACT

A review is presented that covers the experimental and theoretical literature relating to the preparation, electronic structure and chemical and physical properties of the surfaces of the wurtzite form of GaN. The discussion includes the adsorption of various chemical elements and of inorganic, organometallic and organic species. The focus is on work that contributes to a microscopic, atomistic understanding of GaN surfaces and interfaces, and the review concludes with an assessment of possible future directions.

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Abbreviations: 2D, Two-Dimensional; 2DEG, Two-Dimensional Electron Gas; 2DPS, Two-Dimensionally-Periodic Slab; 3D, Three-Dimensional; AES, Auger Electron Spectroscopy; AFM, Atomic Force Microscopy; ARUPS, Angle-Resolved Ultraviolet Photoemission Spectroscopy; B3LYP, Becke-3 Lee-Yang-Parr; BB, Band Bending; BE, Binding Energy; BEP, Beam-Equivalent Pressure; BZ, Brillouin Zone; CBED, Convergent-Beam Electron Diffraction; CBM, Conduction Band Minimum; CMP, Chemo-Mechanical Polishing; C-V, Capacitance-Voltage; CVD, Chemical Vapor Deposition; DB, Dangling Bond; DFT, Density Functional Theory; DFTB, Density Functional Tight Binding; DI, Deionized (H₂O); DOS, Density of States; ECR, Electron Counting Rule; EDAX, Energy-Dispersive Analysis by X-rays; ELS, (Electron) Energy Loss Spectroscopy; ESD, Electron-Stimulated Desorption; FCC, Face-Centered Cubic; FK, Fuchs-Kliewer; FLAPW, Full-Potential Linearized Augmented Plane Wave; GGA, Generalized Gradient Approximation; HCP, Hexagonal Close-Packed; HOMO, Highest Occupied Molecular Orbital; HREELS, High-Resolution Electron Energy Loss Spectroscopy; HRTEM, High-Resolution Transmission Electron Microscopy; HSE, Heyd-Scuseria-Ernzerhoff; IBA, Ion Bombardment and Annealing; IPES, Inverse Photoemission Spectroscopy; ISS, Ion-Scattering Spectroscopy; I-V, Current-Voltage; KE, Kinetic Energy; LDA, Local Density Approximation; LEED, Low-Energy Electron Diffraction; LEEM, Low-Energy Electron Microscopy; MBE, Molecular Beam Epitaxy; MD, Molecular Dynamics; MIGS, Metal-Induced Gap States; ML, Monolayer; MOCVD, Metal-Organic Chemical Vapor Deposition; MOVPE, Metal-Organic Vapor-Phase Epitaxy; NBLP, Non-Bonding Lone Pair (Orbital); NCPP, Norm-Conserving Pseudopotential; NEA, Negative Electron Affinity; NEB, Nudged Elastic Band; NLCC, Non-Linear Core Correction; PAW, Projector Augmented Wave; PBE, Perdew-Burke-Ernzerhoff; PED, Photoelectron Diffraction; PH, Pseudo-Hydrogen; PL, Photoluminescence (Spectroscopy); PP, Pseudopotential; PW, Plane Wave; PW-91, Perdew-Wang 1991; QCO, Quartz Crystal Oscillator; RAS, Reflection-Absorption Spectroscopy; RBS, Rutherford Backscattering; RHEED, Reflection High-Energy Electron Diffraction; RHF, Restricted Hartree Fock; RMS, Root Mean Square; RPES, Resonant Photoemission Spectroscopy; RT, Room Temperature; SAM, Self-Assembled Monolayer; SBH, Schottky Barrier Height; SCL, Space-Charge Layer; SCLS, Surface Core-Level Shift; SE, Spectroscopic Ellipsometry; SIMS, Secondary-Ion Mass Spectroscopy; SPV, Surface Photovoltage (or Surface Photovoltaic); STM, Scanning Tunneling Microscopy; STS, Scanning Tunneling Spectroscopy; SUC, Surface Unit Cell; TEG, Triethylgallium; TEM, Transmission Electron Microscopy; TCE, Trichloroethylene; TMG, Trimethylgallium; TOF-SARS, Time-of-Flight Scattering and Recoil Spectroscopy; TPD, Temperature-Programmed Desorption; UHV, Ultra-High Vacuum; UPS, Ultraviolet Photoemission Spectroscopy; USPP, Ultra-Soft Pseudopotential; UV, Ultraviolet; VBM, Valence Band Maximum; VPE, Vapor-Phase Epitaxy; XAES, X-ray-(Excited) Auger Electron Spectroscopy; XPS, X-ray Photoemission Spectroscopy; XRD, X-ray Diffraction.

[☆]The views presented are those of the author and do not necessarily represent the views of the Department of Defense or its Components.

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