Ab initio simulation of basic processes during growth of gallium nitride by MOVPE method

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Molecular processes of trimethyl gallium (TMG) and its derivatives: DMG and MMG at GaN(0001) surface in MOVPE growth conditions are simulated using ab initio calculations. It is assumed that GAN(0001) surface is covered by mixture of NH_3 admolecules and NH_2 radicals, stabilized by ammonia rich ambient and presence of hydrogen/nitrogen carrier gas. The DFT calculations show the role of methyl gallium derivatives in GaN growth. In the simulations the importance of charge distribution at the surface, electric fields is included. The reaction most probable pathways and the transformations of these chemical species at differently doped gallium nitride Ga polar surface. The stable configurations at the surface, the adsorption sites and the barriers are determined. The possible scenario of methyl groups removal from the surface is proposed. The simulations considerably increase our understanding of the growth mechanism of GaN by MOVPE method.