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Ab initio study of MOCVD synthesis of InN and GaN WERONIKA WALKOSZ[1], Argonne National Laboratory, PETER ZAPOL, MATTHEW J. HIGHLAND, PAUL H. FUOSS, GREGORY B. STEPHENSON — A detailed understanding of MOCVD growth of group III nitrides is important for improved control over their properties and performance in a wide range of applications. Because of the relative instability of InN, chemically active precursors such as NH_3 are typically used to provide the high nitrogen activity needed for growth. Our goal is to understand the mechanism and species involved in active nitrogen formation on the growth surface. Here we present results of density functional theory calculations for the decomposition of NH_3 on InN and GaN (0001) surfaces through reaction intermediates such as adsorbed NH_2 and NH. The calculated equilibrium surface structures along with the reaction barriers for the dissociation pathways of NH_3 on these surfaces are described. Kinetic modeling based on the calculated barriers to determine reaction mechanisms and effective nitrogen activities is discussed. The results will be used to elucidate chemical kinetics on GaN and InN (0001) surfaces under MOCVD growth conditions with the aim to optimize synthesis conditions and precursors for effective growth of metastable nitrides. Work supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

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