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Decomposition of NH_3 and H_2 on ZrB_2 (0001) surface[1]

WERONIKA WALKOSZ, Materials Science Division, Argonne National Laboratory, KEDAR MANANDHAR, MICHAEL TRENARY, Department of Chemistry, University of Illinois at Chicago, PETER ZAPOL, Materials Science Division, Argonne National Laboratory — Group III nitride semiconductors (AlN, GaN, InN, and their alloys) are important materials for applications in solid-state lighting, optoelectronics, and photovoltaics. However, the lack of lattice–matched substrates for their growth results in less than optimal material quality. In the last decade, zirconium diboride (ZrB_2) has been demonstrated as a promising substrate for GaN growth because of its similar lattice constant and thermal expansion properties when compared to the nitride. Moreover, the high electrical conductivity of ZrB_2 makes it desirable for many GaN-based device applications. In this talk, we present results of density functional theory calculations for the reactivity of the $ZrB_2(0001)$ surface towards the N precursor, NH_3, and the carrier gas, H_2, commonly used in metal organic chemical vapor deposition and molecular beam epitaxy of nitrides. Two different terminations of $ZrB_2(0001)$ surface, the Zr and B terminations, are considered and assessed in terms of their catalytic properties toward NH_3 and H_2 decomposition. The theoretical results are analyzed in connection with our recent XPS and RAIRS measurements.

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Weronika Walkosz
Argonne National Laboratory

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