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Effect of surface relaxation and inter-layer interaction on electronic properties of lattice-matched 2D/3D Heterostructures: A first-principles study MAHESH NEUPANE, US Army Rsch Lab - Adelphi, DECARLOS TAYLOR, EDWARD BYRD, US Army Research Lab - Aberdeen, DMITRY RUZMETOV, TERRANCE O'REGAN, TONY IVANOV, US Army Rsch Lab - Adelphi — Transition metal dichalcogenide two-dimensional (2D) materials have shown great potential as next-generation materials for the post-Si era mainly due to their layer-dependent electronic and optical properties. Using these features of 2D materials, many exploratory devices using small-scale exfoliated samples have been designed and studied. Transfer-free large scale growth of 2D materials, however, remains elusive. However, recent large scale growth efforts focusing on defect-free growth of atomically thin 2D materials on 3D substrates such as SiO_2 [1], SiC [2], and GaN [3, 4] have shown some early promise for technologically relevant 2D on 3D growth. Most of these experimental studies highlight the importance of bulk-like surface relaxation in 3D substrates and strong 2D/3D surface interactions during growth. Motivated by these recent experimental advancements, we performed a theoretical/computational study of 2D (MoS_2)/3D (GaN) heterostructure using a first-principle calculation. An attempt will be made to establish a structure-property relationships in the MoS_2/GaN heterostructures by correlating the MoS_2-GaN surface interaction and the electronic properties such as band gap and work-function.1. ACS Nano 2016, 10, 2819-2826; 2. Appl. Phys. Lett 105, 203404, 2014; 3. ACS Nano 2016, 10, 3580-3588; 4. ACS Appl. Mater. Interfaces 2016, 8, 20267−20273.

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