Identifying microscopic mechanisms for hole traps in nitride heterostructures

JOHN LYONS, LUKE GORDON, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Some recent designs of nitride semiconductor devices employ heterostructures (such as N-face high-electron-mobility transistors) in which the electronic Fermi level is established near the valence-band maximum due to the influence of polarization fields. In many of these heterostructures, the presence of hole-trapping centers is thought to adversely affect device performance. This behavior has been observed in many different types of devices, and its physical origin remains unknown. Using first-principles calculations based on a hybrid functional, we investigate possible origins for this phenomenon. We explore both intrinsic defect candidates as well as impurities. With Schrödinger-Poisson simulations, we then investigate how the behavior of these species and their spatial distribution within the heterostructure layers is reflected in the performance of nitride semiconductor devices.

This work was supported by the DEFINE MURI.