Abstract Submitted
for the 4CS21 Meeting of
The American Physical Society

Engineering Defects in AlGaN for Advanced Information Processing JEREMY KAMIN, New Mexico State University, DR. JULIA DEITZ, Sandia National Laboratories, DR. BORIS KIEFER, New Mexico State University
— It is well known that defects can fundamentally change the electronic structure of materials and thereby enable novel applications. For example, point defects in diamond (NV-centers) create novel electronic states with uses in quantum computing and quantum sensing. However, diamond is costly and comparatively difficult to manipulate. Here we report on density-functional-theory (DFT) assessment of point defects in AlN, AlGaN, and GaN and their effect on electronic, magnetic, and optical properties. Dopants were selected by minimizing ionic radii mismatch with Al and Ga, low spin-orbit coupling and high abundance of (nuclear) spin-singlet isotopes. Among the most promising elements are Si and Cr. Our preliminary results show that Gavacancies alone may be beneficial for spin-qubit design. Combining Si-dopant and Ga-vacancy may be beneficial for robust spintronics. Similarly, Cr doping may find application in spin-based devices and technologies. Therefore, defect engineering in widegap insulators appears as a unifying materials platform that can support a wide range of spin-based technologies. Sandia National Laboratories are managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Jeremy Kamin
New Mexico State University

Date submitted: 10 Sep 2021 Electronic form version 1.4