Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles studies of electron transport in Ga_2O_3[1]
YOUNGHO KANG, KARTHIK KRISHNASWAMY, HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara — Ga_2O_3 is a wide-gap semiconductor with a monoclinic crystal structure and a band gap of 4.8 eV. Its high carrier mobility and large band gap have attracted a lot of attention for use in high power electronics and transparent conductors. Despite its potential for adoption in these applications, an understanding of its carrier transport properties is still lacking. In this study we use first-principles calculations to analyze and compute the electron scattering rates in Ga_2O_3. Scattering due to ionized impurities and polar longitudinal-optical (LO) phonon is taken into account. We find that the electron mobility is nearly isotropic, despite the low-symmetry monoclinic structure of Ga_2O_3. At low carrier densities ($\sim 10^{17}$ cm^{-3}), the mobility is limited by LO phonon scattering. Scattering by ionized impurities becomes increasingly important at higher carrier densities. This type of scattering is enhanced when compensating native point defects are present; in particular, gallium vacancies, which are triply negatively charged, can have a strong effect on mobility. These effects explain the downturn in mobility observed in experiments at high carrier densities.

[1]This work was supported by ARO and NSF.

Youngho Kang
Univ of California - Santa Barbara

Date submitted: 09 Nov 2016 Electronic form version 1.4