Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Near-edge optical properties of β-Ga_2O_3 determined through first-principles calculations[1] KELSEY MENGLE, GUANGSHA SHI, DYLAN BAYERL, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — $\beta-Ga_2O_3$ is a wide band-gap material of interest for many applications, including high-power electronics and optoelectronics. The electronic and optical properties are especially interesting due to its wide band gap, reported in the literature between 4.4-5.0 eV. We use first-principles calculations including density functional theory (DFT) and many-body perturbation theory (GW) to investigate the discrepancy in the reported values of the fundamental band gap and whether the nature is direct or indirect. We find that the band gap is indirect but only 29 meV lower in energy than the direct gap. By comparing the imaginary part of the dielectric function to the calculated optical matrix elements for Γ—Γ electronic transitions, we verify the directional-dependence of the absorption onsets for the material. This anisotropy can explain the broad range of reported band gaps. The calculated radiative recombination coefficients demonstrate that despite being an indirect-gap material, intrinsic deep-UV light emission is possible with β-Ga_2O_3 at high excitation.

[1]This research was supported by the National Science Foundation through Grant No. DMR-1534221 and the GRFP through Grant No. DGE 1256260. Computational resources were provided by the DOE NERSC facility under Contract No. DE-AC02-05CH11231.

Kelsey Mengle
Univ of Michigan - Ann Arbor

Date submitted: 10 Nov 2016 Electronic form version 1.4