Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Optoelectronic properties of Ta_3N_5: A joint theoretical and experimental study[1] JULIANA MORBEC, Institute for Molecular Engineering, University of Chicago, USA, IEVA NARKEVICIUTE, THOMAS JARAMILLO, Department of Chemical Engineering, Stanford University, USA, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago, USA — A joint theoretical and experimental study of the optoelectronic properties of Ta_3N_5 was conducted by means of ab initio calculations and ellipsometry measurements [1]. Previous experimental work on Ta_3N_5 has not been conclusive regarding the direct or indirect nature of light absorption. Our work found excellent agreement between the optical spectrum computed using the Bethe-Salpeter equation and the measured one, with two prominent features occurring at 2.1 and 2.5 eV assigned to direct transitions between N and Ta states. The computed optical gap, obtained from the G_0W_0 direct photoemission gap, including spin-orbit coupling, electron-phonon interaction, and exciton binding energy, was found to be in excellent agreement with measurements. Our results also showed that Ta_3N_5 is a highly anisotropic material with heavy holes in several directions, suggesting low hole mobilities, consistent with low measured photocurrents in the Ta_3N_5 literature. Work is in progress to compute polaronic contributions to the hole and electron mobilities and to investigate the effect of substitutional doping on the electronic structure of Ta_3N_5.

[1] Juliana M. Morbec, Ieva Narkeviciute, Thomas F. Jaramillo, and Giulia Galli, Phys. Rev. B 90, 155204 (2014).

[1]Work supported by NSF (NSF Center CHE-1305124 for CCI Solar Fuels). Computing resources provided by NERSC.

Juliana Morbec
Institute for Molecular Engineering, University of Chicago, USA

Date submitted: 07 Nov 2014 Electronic form version 1.4