Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Structural and electronic properties of $ZnGeN_2$[1] NICHOLAS L. ADAMSKI, Department of Electrical and Computer Engineering, University of California, Santa Barbara, California 93106-9560, USA, ZHEN ZHU, DARSHANA WICKRAMARATNE, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, California 93106-5050, USA — $ZnGeN_2$ is a direct-band-gap earth-abundant semiconductor that is a candidate material for photovoltaic and light-emitting devices. Elucidating the potential use of $ZnGeN_2$ in such applications requires an accurate knowledge of its structural and electronic properties, as well as an understanding of the role of native point defects in the material at the microscopic level. Using density functional theory with a hybrid functional, we study the structural and electronic properties of $ZnGeN_2$. We investigate the role of native point defects, specifically antisites, vacancies and interstitials, and discuss their impact on electronic and optical properties.

[1]This work is supported by ARO.

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Date submitted: 10 Nov 2016 Electronic form version 1.4