Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic and Optical properties of Vacancy Defects in two dimensional monolayer Transition metal Dichalcogenides MAHTAB KHAN, MIKHAIL EREMENTCHOUK, MICHAEL LEUENBERGER, University of Central Florida — Defects play an important role in tailoring electronic and optical properties of two-dimensional monolayer transition metal dichalcogenides (TMDCs). Recently it has been shown that the presence of vacancy defects (VDs) in two-dimensional monolayer MoS_2 induces localized states which give rise to extra resonance peaks in both in-plane $\chi_{\parallel}$ and out-of-plane $\chi_{\perp}$ susceptibilities.[1] In-plane $\chi_{\parallel}$ and out-of-plane $\chi_{\perp}$ susceptibilities are related to the presence of even and odd states with respect to the Mo plane, respectively[1]. Moreover, monolayer TMDCs have a large spin orbit coupling (SOC), originating from d-orbitals of heavy transition metals and being of the order of a few 100 meV. We present a more general picture of the electronic and optical properties of defected monolayer TMDCs. In particular, we consider MoS_2, $MoSe_2$, WS_2 and WSe_2 with three types of VDs (i) Mo, W vacancy, (ii) S_2, Se_2 vacancy, and (iii) S, Se vacancy. In addition, we investigate the effects of SOC on the band structures and the optical susceptibilities of VDs in TMDCs.
1. Mikhail Erementchouk, M. A. Khan, and Michael N. Leuenberger, Phys. Rev. B 92, 121401(R) (2015).

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Date submitted: 06 Nov 2015 Electronic form version 1.4