Michael N Leuenberger et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

conferenceseries.com

3rd International Conference on

Smart Materials & Structures

March 20-22, 2017 Orlando, USA

Electronic and optical properties of transition metal dichalcogenides in the presence of vacancy defects

Michael N Leuenberger[1], **M A Khan**[1,2], **Mikhail Erementchouk**[1,3] and **Joshua Hendrickson**[4]
[1]University of Central Florida, USA
[2]Federal Urdu University of Arts, Science and Technology, Pakistan
[3]University of Michigan, USA
[4]Air Force Research Laboratory-Wright-Patterson Air Force Base, USA

Single layer (SL) transition metal dichalcogenides (TMDCs) (MX_2; M=transition metal such as Mo, W and X= S, Se, Te) have attracted a lot of attention due to their intriguing electronic and optical properties. SL TMDCs are direct band gap semiconductors, which can be used to produce smaller and more energy efficient devices such as transistors and integrated circuits. Moreover, the band gap lie in the visible region, which makes them highly responsive when exposed to visible light, a property with potential applications in optical detection. In contrast to graphene, SL TMDCs exhibit large spin-orbit coupling (SOC) originating from the d orbitals of the transition metal atoms. The presence of the giant SOC makes them great candidates for exploring spin physics and for spintronic devices. Defects usually play an important role in tailoring electronic, optical and magnetic properties of semiconductors. We performed standard first-principle study to evaluate the electronic and optical properties of single-layer (SL) transition metal dichalcogenides (TMDCs), in the presence of vacancy defects (VDs). We consider three types of VDs in SL TMDCs (1) X-vacancy, (2) X_2-vacancy, and (3) M-vacancy. We find that VDs lead to localized defect states (LDS) in the band structure, which in turn give rise to sharp transitions in in-plane and out-of-plane optical susceptibilities, $\chi\Pi$ and $\chi\perp$, respectively. The effects of spin orbit coupling (SOC) are also considered. We find that SOC splitting in LDS is directly related to the atomic number of the transition metal atoms. Apart from electronic and optical properties we also find magnetic signatures (local magnetic moment of $\sim\mu_B$) in $MoSe_2$ in the presence of Mo vacancy, which breaks the time reversal symmetry and therefore lifts the Kramers degeneracy. We use group theory to derive the optical selection rules for both $\chi\Pi$ and $\chi\perp$.

Biography

Michael N Leuenberger has received his PhD degree in Theoretical Physics in 2002 from the University of Basel in Switzerland. After his Postdoctoral positions at the University of Iowa and at the University of California, San Diego he joined in 2005 the NanoScience Technology Center at the University of Central Florida and became tenured Associate Professor in 2011. In 2008, he has received the DARPA/MTO Young Investigator Award. His current research areas include quantum information processing in topological insulators, optoelectronics in 2D materials and solar energy harvesting in nanoparticles. He has published more than 60 peer-reviewed papers and 4 book chapters.

michael.leuenberger@ucf.edu

Notes: