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Optical signatures of states bound to vacancy defects in monolayer transition metal dichalcogenides

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The non-zero thickness of transition metal dichalcogenide (TMDC) single layer (SL) manifests in electron states forming classes of states even and odd with respect to reflections through the central plane. These states are energetically well separated and give rise to two bandgaps $E_{g||}$ and $E_{g\perp}$ for the optical in-plane and out-of-plane susceptibilities $\chi_{||}$ and $\chi_{\perp}$ respectively. Because of this, odd states are often neglected, which effectively reduces TMDC SL to a perfect 2D system. We study states bound to various vacancy defects in TMDC SL and show that odd states play an equally important role as even states. In particular, we show that odd states bound to VD lead to resonances in $\chi_{\perp}$ inside $E_{g\perp}$ in TMDC SL with VDs. Additionally, we demonstrate that the states bound to VDs are not necessarily confined to the bandgap in the even subsystem, which requires the extension of the energy region affected by the bound states. The resulting optical signatures not only provide the possibility to identify the type but also the concentration of VDs, thereby paving the way to quantifying the purity of defected TMDC SL containing VDs.

Biography

Michael N Leuenberger received his PhD 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 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.

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