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Defect activated optical Raman modes in single layer $MoSe_2$

MAIA OFREDI CARDOSO Fábio[1], MACIEL OLIVEIRA Indhira[2], MASSOTE PAZZINI VASCONCELOS Daniel[2], ARCHANJO SOARES Braulio[3], LEGNANI Cristiano[2], QUIRINO GIANINI Welber[2], LACERDA GRIBEL Rodrigo[1], CAROZO Victor[4], FRAGNEAUD Benjamin[2]

[1]Departamento de Física, Universidade Federal de Minas Gerais (UFMG), Belo Horizonte, MG, Brasil
[2]Departamento de Física, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora, MG, Brasil
[3]Divisão de Metrologia de Materiais, Instituto Nacional Metrologia (INMETRO), Rio de Janeiro, RJ, Brasil
[4]Departamento de Física, Pontifícia Universidade Católica (PUC-RJ), Rio de Janeiro, RJ, Brasil

offredifabio@gmail.com; indhira@fisica.ufjf.br; massote@ice.ufjf.br; bsarchanjo@inmetro.gov.br; cristiano.legnani@ufjf.br; rlacerda@fisica.ufmg.br; wgquirino@ice.ufjf.br; vcarozo@puc-rio.br; benjamin.fragneaud@ice.ufjf.br

Abstract

TMDs have been intensively synthesized/studied thus linking their morphological aspect to their physical properties, and consequently leading to the understanding of the possible benefits of defects in such materials. Nevertheless, for future applications, quantifying and identifying defects in TMDs is still a milestone to reach in order to better employ these materials in optoelectronic devices. Raman Spectroscopy has been successfully employed in graphene to quantify punctual or line defects. In this work [2], we bombarded monolayer $MoSe_2$ with He ions and found out the existence of three defect activated Raman bands around 250–300 cm^{-1}. DFT calculations were employed to obtain the electronic and phonon dispersion bands, making it possible to infer that these bands arise from inter-valley Raman double resonance processes. Interestingly, the same punctual defect model, that allows one to predict the defect concentration at which graphene starts to become amorphous, also works for TMDs. Hence, this work opens the door to the macroscopic quantification of defects in TMDs, which is essential for technological applications.

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