Raman Investigation of Defective Monolayer MoS2 from First-principle Calculations

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Direct band gap of 1.8 eV, spin-orbit coupling, and high Seebeck coefficient are couple of examples that why monolayer MoS2 is currently being object of great attention. Like all real materials, the monolayer of MoS2 contains some structural defects that can be detrimental or beneficial depending on the targeted application. Raman spectroscopy technique is a powerful tool for the characterization of the quality of 2D structures. In this context, we compare Raman spectra of different common defects in monolayer MoS2 like vacancy, substitution, and adatom. We also study Raman spectra as a function of defect concentration. In addition to the unfolded phonon spectra are presented.

References

[1] Wenting Zhang, Xiaodong Li, Tongtong Jiang, Jiangluqi Song, Yue Lin, Lixin Zhu and Xiaoliang Xu, Nanoscale, 2015, 7, 13554-13560.

[2] Elisha Mercado, Andy Goodyear, Jonathan Moffat, Mike Cooke and Ravi S Sundaram, J.Phys. D: Appl. Phys. 2017. 50, 184005.

[3] Klein, A Kuc, A Nolinder, M Altzschner, J Wierzbowski, F Sigger, F Kreupl, J J Finley, U Wurstbauer, A W Holleitner,and M Kaniber 2D Mater,2018, 5, 011007.

Figures

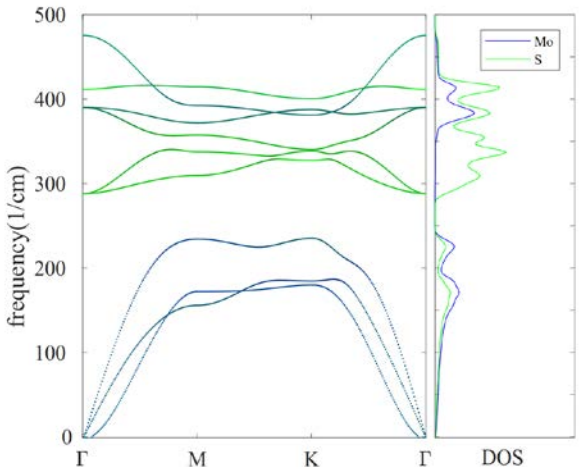

Figure 1: Phonon dispersion curve together with partial phonon DOS for monolayer MoS2.

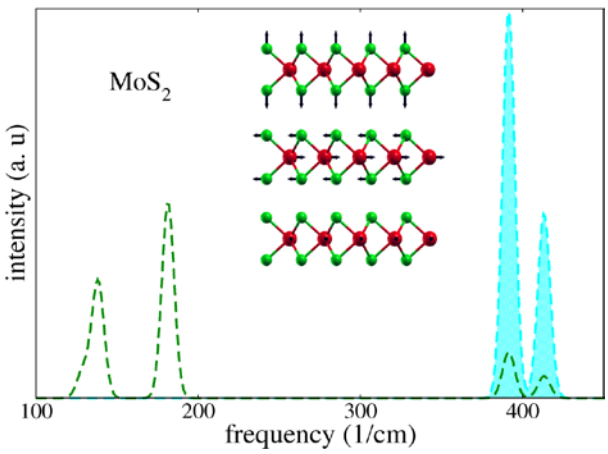

Figure 2: Unpolarized Raman spectra for MoS2 in weighted (shaded regions) and bare (dash line) forms.