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DOUBLE RESONANT RAMAN SCATTERING IN TMDCS

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Raman spectra of TMDCs have been reported for several decades. The first-order Raman process in TMDCs has been widely investigated and is now well understood. However, the study of second-order Raman spectra did not yet give consistent assignments for different TMDCs. We study the second-order Raman process of monolayer TMDCs, by combining *ab initio* density functional perturbation calculations with experimental Raman spectroscopy and electron-phonon Wannier (EPW) method [1-4]. The calculated electronic band structure and the density of states show that the resonance Raman process occurs at the M point in the Brillouin zone (**Figure 1**), where a strong optical absorption occurs due to a logarithmic Van Hove singularity of the electronic density of states. The double resonance Raman process with intervalley electron-phonon coupling connects two of the three inequivalent M points in the Brillouin zone, giving rise to second-order Raman peaks due to the M-point phonons. The calculated vibrational frequencies and laser-energy dependent Raman spectra of the second-order Raman spectra agree with the observed laser-energy-dependent Raman shifts in the experiment. We also predicted the helicity dependence of the double resonant Raman modes.

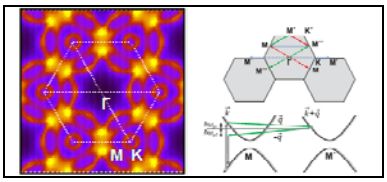

Figure 1. (left) Optical absorption in the Brillouin zone at a certain laser energy. (right) The schematics of the double resonance process (electron-photon and electron-phonon processes).

References

[1] H. Guo, T. Yang, M. Yamamoto, L. Zhou, et al., Phys. Rev. B **91**, 205415 (2015).
[2] Hsiang-Lin Liu, Huaihong Guo, et al., Phys. Chem. Chem. Phys. **17** (22), 14561 (2015).
[3] R. Saito, A. R. Nugraha, E. H. Hasdeo, S. Siregar, Huaihong Guo, Teng Yang, Physica Status Solidi B **252** (11), 2363–2374 (2015).
[4] Hsiang-Lin Liu, Teng Yang, Yuki Tatsumi, Ye Zhang, Baojuan Dong, Huaihong Guo, Zhidong Zhang, Yasuaki Kumamoto, Ming-Yang Li, Lain-Jong Li, Riichiro Saito, Satoshi Kawata, Scientific Reports **8**, 11398 (2018).