Electronic Structure Study of Intercalated Transition Metal Dichalcogenide

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Abstract. Intercalated transition metal dichalcogenide (TMDCs) has recently attracted attention of condensed matter community owing to the exhibition of the exotic phenomena depending upon the intercalate transition metal [1]. We explore the electronic structure of V-intercalated TMDCs $V_{1/3}NbS_2$ using spin and angle resolved photoemission spectroscopy (SARPES) in combination with one step model of photoemission as implemented in the SPR-KKR package [2], our calculations can combine temperature- and phonon energy-dependent effects via inclusion of both bulk and surface phonons. Raman spectroscopy has been also employed to observe the signature of intercalated metal monolayer in the samples. For determining bulk as well as surface lattice structure of the $V_{1/3}NbS_2$ monocrystals, we have utilized multiple characterizations techniques Low electron energy diffraction (LEED) and single crystal X-ray diffraction. Our structural measurements show high quality crystals exhibiting P6₃22 space group. Comparison of band structure measurements and calculations shows unidentified features in the measured band structure.

REFERENCES

1. B. Edwards et al, Nature Materials 22, 459 (2023)

2. H. Ebert, D. Ködderitzsch and J. Minár, Rep. on Prog. in Phys. 74, 096501 (2011)