The CD-ARPES Study of Intercalated Transition Metal Dichalcogenide $V_{1/3}NbS_2$

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Abstract. Transition metal dichalcogenides (TMDCs) have garnered significant attention from the condensed matter community due to the demonstration of a wide spectrum of future technologically important properties such as super conductivity, charge density waves. Their 2H-polytype is characterized by weak van der Waals interactions between adjacent layers, offers a unique platform for manipulation and tuning of physical properties. Among the various strategies to engineer their functionalities, **intercalation of transition metal ions** stands out as a particularly powerful approach. This intercalation not only modifies the interlayer coupling but can also introduce new degrees of freedom, such as localized magnetic moments or charge transfer effects. **Intercalating transition metal ions into transition metal dichalcogenides (TMDCs)** such as NbS_2 can elicit long-range magnetic order and can host a variety of non-trivial spin textures. In specific compositions such as $M_{1/3}NbS_2$, intercalated atoms adopt ordered superstructures, where intercalants occupy specific sites-ideally the **2c Wyckoff position**, above and below each NbS_2 layer. This ordered arrangement breaks the global inversion symmetry and transitioning the crystal from the **centrosymmetric $P6_3/mmc$** (typical of $2H\text{-}MX_2$) to the **non-centrosymmetric $P6_322$** space group. Non-centrosymmetry significantly influences the **magnetic interactions** between intercalated atoms. Thus considered to be essential to supplementary for exploring exotic phenomena like altermagnetism, chiral spin textures, and nonlinear optical responses. Among these systems, V-intercalated compounds are of special interest. Symmetry-group theoretical predictions suggest that $V_{1/3}NbS_2$ exhibits **altermagnetism**—a magnetic state where collinear spins break time-reversal symmetry (TRS) in the band structure, yet do not yield a net magnetization. However, in $M_{1/3}NbS_2$, intercalants may also occupy multiple potential sites, leading to **site disorder**, which can affect magnetic transition temperatures and even **restore centrosymmetry**. Therefore, this research includes a focused investigation into the role of **site disorder** on the **magnetic and electronic structure properties** of otherwise non- centrosymmetric system.

In this work, we have synthesized $V_{1/3}NbS_2$ single crystals and studied structural, magnetic and electronic structure properties. We aim to further understand the role of **site disorder** on the **magnetic and electronic structure properties** of otherwise non-centrosymmetric system V-intercalated TMDC, $V_{1/3}NbS_2$ using Circular Dichroic Angle-Resolved Photoemission Spectroscopy (CD-ARPES) in combination with the one-step model of photoemission as implemented in the SPR-KKR package.