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Charge density study of van der waals-layered MoS_2 and TiS_2

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High-resolution diffraction data are essential to determine accurate charge density. We reported d-space resolution dependence of the charge densities in Ref. 1. To obtain high-resolution X-ray diffraction data, we have performed synchrotron diffraction experiments using 60 keV X-ray at PETRA-III [2], 50 keV X-ray at SPring-8 and multiple powder diffraction data method [1]. Recently, we have probed charge densities of iso-structural metal hexaborides as a pi-bonding system using ultra-high resolution d > 0.22 Å powder data [3]. Our present challenge is to evaluate the weak interaction in van der Waals-layered structures such as MoS_2 and TiS_2. The layered transition metal dichalcogenides have been attractive due to their unique properties, e.g., as topological insulators, charge density wave system and materials for energy. The layered structure exhibits strong covalent intralayer bonding and weak van der Waals (vdW) interlayer interaction. Compared to strong intralayer bonding, weak interlayer interaction is difficult to be evaluated not only experimentally but also theoretically because vdW force is not described in ground states. The experimental evaluation of vdW interlayer interaction can be useful for the fundamental understanding of the vdW interaction and layered structure. In the present study, we evaluate and compare the weak vdW interlayer interaction in MoS_2 (space group: $P6_3/mmc$) and TiS_2 (space group: $P\text{-}3m1$) using experimental X-ray charge densities. The charge densities were modelled with the Hansen-Coppens multipole model using single-crystal diffraction data with a resolution of d > 0.3 Å measured at the BL02B1 of SPring-8. In the presentation, we will discuss the weak interlayer vdW interaction from experimental and theoretical charge densities.

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[2] Tolborg, K. et al. (2017). Submitted.
[3] Kasai, H. & Nishibori, E. (2017). Sci. Rep. **7**, 41375.

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