Electron Density of a Layered Transition Metal Dichalcogenide

Hidetaka Kasai1,2, Kasper Tølbøll3, Mattia Sistrø2, Venkatesha R. Hathwar2, Mette O. Filsoe2, Simone Cenedese5, Kunihisa Sugimoto1, Jacob Overgaard2, Eiji Nishibori3, Bo B. Iversen2

1. Faculty of Pure and Applied Sciences, TIMS and CiRSE, University of Tsukuba
2. Center for Materials Crystallography, Department of Chemistry and iNANO, Aarhus University
3. Japan Synchrotron Radiation Research Institute

Email: kasai.hidetaka@chem.au.dk

Electron density (ED) studies enable us to understand chemical bonding features in materials. While accurate experimental ED has provided information on bonding in a variety of materials, it is still a great challenge to evaluate weak interactions e.g. in layered structures. Layered transition metal dichalcogenides (TMDs) have attracted much attention because of their unique properties e.g. as topological insulators [1], charge density wave systems [2], electrode materials for ion batteries [3], and thermoelectric materials [4]. The generalized formula is $\text{MX}_2$, where M is a transition metal and X is a chalcogen (S, Se and Te). The layered structure exhibits strong covalent intralayer bonding and weak van der Waals (vdW) interaction between adjacent layers. The weak vdW interaction also enables stacking different TMDs layers [5] as well as application of a monolayer or a few-layer TMDs [6]. Understanding the weak interaction in TMDs is important not only for fundamental science but also for application. Recently the interlayer interaction in SnS$_2$ was discussed using high pressure techniques [7]. In the present study, we evaluate the weak interlayer interaction in TMDs using experimental X-ray ED. We measured single crystal diffraction data of TiSe$_2$ (Space Group: $P\overline{3}m1$) to a resolution of $\sin \theta / \lambda = 1.67$ Å$^{-1}$ at 20 K using 50 keV X-ray with the image plate detector at BL02B1 of SPring-8. The ED was modelled with the extended Hansen-Coppens multipole model [8], which includes refinement of core electron density features. In the presentation, we will discuss the weak interlayer interaction based on the ED.


Keywords: Electron density, layered structure, multipole model