Investigations of the atomic electric field and charge density distribution in 2D WSe2 by high resolution STEM Differential Phase Contrast imaging and DFT

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2D materials are currently subject of intensive research in various fields due to their interesting optoelectronic properties, which are strongly influenced by the internal electric field and the charge density distribution. Due to the inherently low dimensionality of 2D materials, defects such as vacancies or impurities can significantly change the field distribution and thus the optoelectronic properties. This makes a precise fabrication of defects in 2D materials particularly interesting for tailored optoelectronic applications. Due to their tunable band gap in the visible range, transition metal dichalcogenides (TMD) are, for example, of great interest for single photon emission induced by defects in the material [1,2]. TMDs consist of molecular layers with the stochiometric form MX2 (M: transition metal, X: chalcogenide) which are bound to each other only by weak van-der-Waals interaction. Spectroscopic methods provide a detailed insight into the electronic properties of these materials. However, they are limited by their spatial resolution, which makes it difficult to investigate the influence of individual defects on the electric field distribution. Only few techniques allow for studying the internal electric field with such a high spatial resolution. Among these techniques is high-resolution differential phase contrast (DPC) imaging in the scanning transmission electron microscope. In DPC, electric fields can be measured with subatomic resolution by detecting the shift of the centre of mass (CoM) of the intensity distribution of the electron beam with a position sensitive detector. The shift of the CoM is caused by the interaction of the beam electrons with the electric potential in the material [3].We investigate the electric field and charge density distribution of mechanically exfoliated 2D WSe2 using DPC. The DPC measurements are performed in an aberration-corrected STEM using a low acceleration voltage of 80 kV and an eight-fold segmented bright-field detector. Images are compared with multislice image simulations performed for the present experimental conditions. The atomic electric field and charge density distributions in pristine mono- and multilayers of WSe2 are presented. Investigations of a vacancy-type defect at Se columns in the 2D material indicate a characteristic change in the electric field distribution, which is revealed by comparing the DPC images of pristine and defective WSe2 samples. A relaxation of the neighboring W atomic columns towards the defect site is observed and confirmed by DFT simulations.

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