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ABSTRACTS

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Probing the interlayer coupling in two-dimensional layered 2H-MoS2 and 2H-WS2 by EXAFS and reverse Monte Carlo simulations

Dr Inga Pudza[1], Dr Andris Anspoks[1], Dr Aleksandr Kalinko[2], Dr Edmund Welter[2], Dr Alexei Kuzmin[1]

[1]Institute of Solid State Physics, University of Latvia, [2]Photon Science – Deutsches Elektronen-Synchrotron (DESY)

Two-dimensional (2D) layered materials, including transition metal dichalcogenides, have attracted considerable interest during the last decades due to their extraordinary electronic, optical, transport, and tribological properties. The structure of these materials is characterized by strong in-plane covalent chemical bonds and weak van-der-Waals (vdW) interactions between layers. When the thickness of layered material is reduced to a single or only a few layers, their electronic and optical properties are strongly affected due to the quantum confinement effect. Thus, interlayer coupling represents a unique degree of freedom to control the properties of 2D materials and their applications in devices.

X-ray absorption spectroscopy (XAS) has been used in the past to probe the short-range order in 2D materials. However, the conventional approach to XAS data analysis, based on multi-shell modeling, cannot provide reliable information on the long-range (across the vdW spacing) interlayer interactions due to a strong correlation between model parameters for distant coordination shells. At the same time, the extraction of such information is possible using an advanced approach, since the range of atomic structure around the absorbing atoms probed by XAS extends up to 10-15 Å, being limited by the photoelectron mean-free path.

In this study, we demonstrate the possibility to extract temperature dependence (10-300 K) of intralayer and interlayer interactions in 2D 2H-MoS_2 and 2H-WS_2 from the analysis of the Mo K-edge and W L_3-edge EXAFS spectra using the reverse Monte Carlo (RMC) simulations. The analysis performed up to the tenth coordination shell allowed evaluation of EXAFS sensitivity to interactions between atoms located in different layers. We found that the mean-square relative displacement factors for atom pairs located in the same or neighboring layers differ significantly indicating a drastic reduction of correlation between distant atoms.

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