Theoretical studies of transition metal dichalcogenides for the use in electron holography — •Sven Borghardt[1], Zeila Zanolli[4], Matthieu Verstraete[3], Florian Winkler[2], Juri Barthel[2], Rafal Dunin-Borkowski[2], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany — [3]PCPM, Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [4]PGI-2 and IAS, Forschungszentrum Jülich, Jülich, Germany

Few-layer transition metal dichalcogenides (TMDs) represent a new family of materials with promising properties for new optoelectronic nano-devices. Their well-known and tailorable thickness render them an ideal system for quantitative electron holography.

Here, we present the simulation of the effect of charge reorganisation due to bonding on the phase acquired by electrons passing through few layer TMD structures in electron holography experiments. This is done by simulating the phases for potentials from density functional theory calculations in comparison with ones obtained from the independent-atom approximation. The results show in an impressive way that neglecting the atomic bonding and the associated small change in the overall charge distribution leads to an overestimation of the average electron phase by approximately 5% for the analyzed materials. Comparison with experimental data confirms this conclusion.

Building on the results for pristine materials, we present calculations for single defects and heterostructures composed of different materials from the transtition-metal dichalcogenide family.