Defects and edges in metal chalcogenide layers

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In addition to Graphene 2D transition metal chalcogenide, as for example MoS2 and WS2, nanostructures are promising materials for applications in electronics and mechanical engineering. Though the structure of these materials results in a highly inert surface with a low defect concentration, defects and edge effects can strongly influence the properties of these nanostructures. Therefore, a basic understanding of the interplay between electronic and mechanical properties and the influence of defects and edge states is needed. We demonstrate on the basis of atomistic quantum mechanical simulations of several types of MoS2 nanostructures how the edge structure and defects influence the mechanical behavior, the electronic properties of such systems.