

# Defects and Edges in Molybdenum Disulfide Layers

---

Gotthard Seifert<sup>1</sup>

Jan-Ole Joswig<sup>1</sup>, Tommy Lorenz<sup>2</sup> and Andre Niebur<sup>1\*</sup>

---

<sup>1</sup>Theoretische Chemie, Technische Universität Dresden, 01062 Dresden, Germany

<sup>2</sup>Technische Thermodynamik, Technische Universität Dresden, 01062 Dresden, Germany

\*Present address: Leibniz Universität Hannover, Institut für Physikalische Chemie und Elektrochemie, Callinstr. 3A, 30167 Hannover, Germany

[gotthard.seifert@tu-dresden.de](mailto:gotthard.seifert@tu-dresden.de)

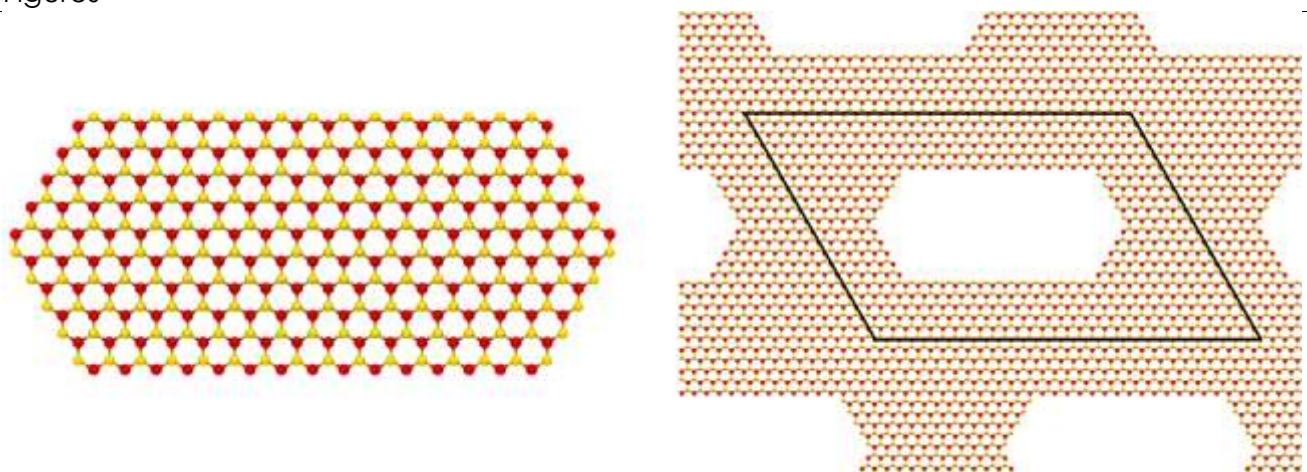
---

In addition to Graphene, 2D transition-metal chalcogenide, as for example MoS<sub>2</sub> and WS<sub>2</sub>, 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 the material. 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 systematic density-functional based study, how the edge structure and defects influence the mechanical behavior and the electronic properties of such systems. We investigated a broad variety of different types of defects and studied the influence of defect sizes and distances between defects. As result of the calculations, the energetic and the electronic properties of defective MoS<sub>2</sub> monolayers can be viewed as a combination of edge and bulk properties with the defect size being of dominating influence. The influence of the defect-edge termination on the electron localization for defects and corresponding finite particles are discussed – see Fig. 1. Finally, the consequences of the defect states on electron transport properties are shown.

---

Figures



**Figure 1:** left: hexagonal MoS<sub>2</sub> plate, right: periodic MoS<sub>2</sub> monolayer with a hexagonal defect in the shape of a plate with indicated unit cell.