MoS_2 Nanostructures: Semiconductors with metallic edges

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We present theoretical simulations based on Density-Functional Theory (DFT) for MoS_2 nanoribbons. We calculate electronic band structure and use linear-response theory to simulate the optical absorption of the material via dielectric function calculations.In addition, we calculate optoelectronic properties such as static relative permittivity, refractive index and reflectivity. Calculations are performed with the Grid-based Projected Augmented Wave (GPAW) package.

By studying nanoribbons with different widths, a single layer MoS_2 and bulk MoS_2 , we observe that the electronic and optical properties of the material depend strongly on the dimensionality. The static relative permittivity drops from 7.1 in 3D to 3.7 in 2D, consistent with experimental data, and down to 2.4 for the quasi-1D nanoribbon. This dramatic change in optoelectronic properties is attributed to the presence of metallic edges in the 1D MoS2, an otherwise semiconducting material (see Fig. 1). By studying nanoribbons with different widths, we are able to provide quantitative characteristics of these quasi-metallic states such as their spatial extent and permittivity [1].

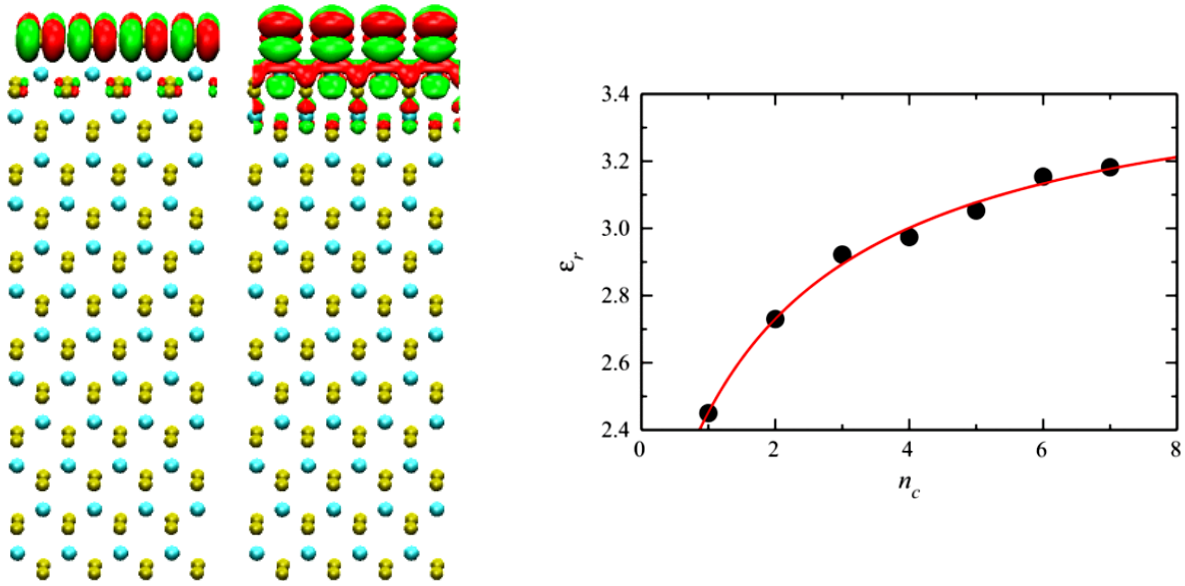

Figure 1:**left:** Isosurfaces of the electronic wavefunctions at the HOMO (left) and the LUMO state (right) for a nanoribbon with a width of n_c=6 cells. Mo and S atoms are represented by blue and yellow spheres, respectively. Different colors correspond to different sign of the wavefunction**.right:**Static relative permittivity as a function of nanoribbon width.

Acknowledgment: This work is supported by the research committee of the Univeristy of Crete.

Reference

[1] D. Davelou, G. Kopidakis, G. Kioseoglou and I. N. Remediakis , Solid State Commun. **192** 42 (2014)