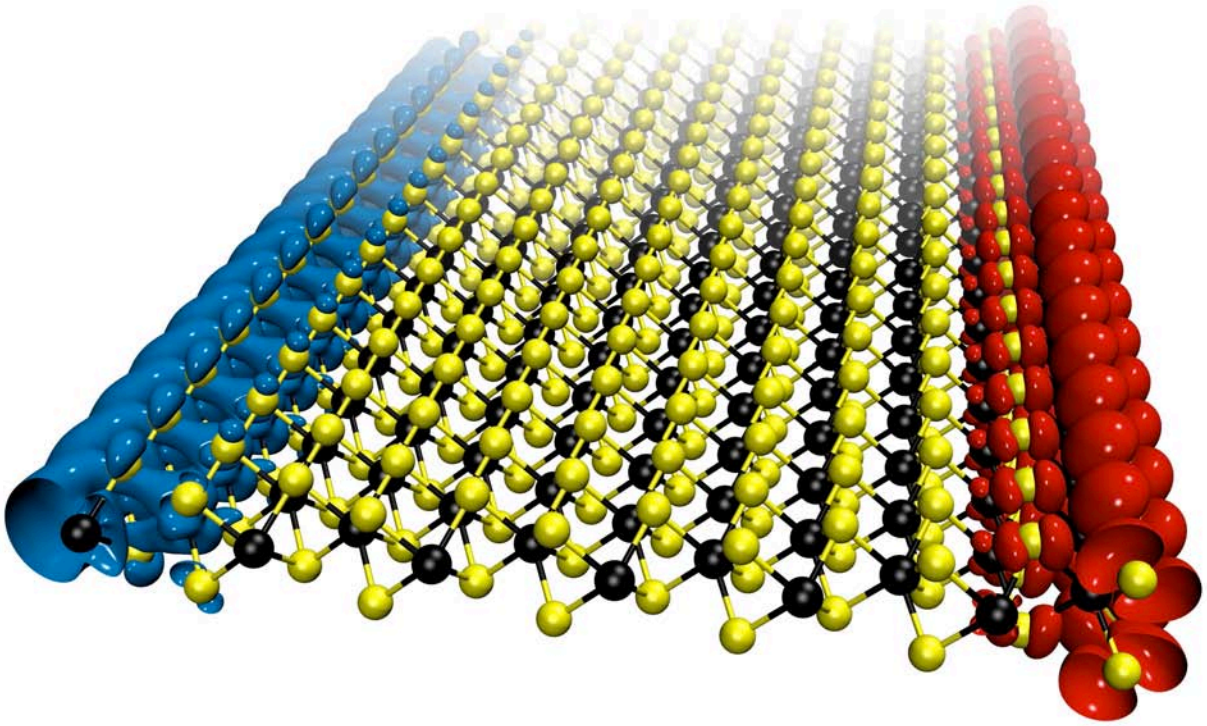

2017 ACCES Visualization Contest - Example B

Entry title: *1D electron and hole wires at the edges of a MoS_2 nanoribbon*
Group members: *Marco Gibertini (post-doc, THEOS)*
Category: *Static*

Computational Thinking

One-dimensional wires of free carriers emerge at interfaces and edges of two-dimensional polar materials. The following procedure has been adopted to numerically predict their existence and visualize their spatial profile.

Abstraction

When a polar two-dimensional (2D) material is cut into a finite-width stripe (*i.e.* a nanoribbon), polarization charges appear at the edges and create electric fields that drive a charge reconstruction. As a net result, one-dimensional wires of free electrons and holes appear at the edges and could enable applications in electronics, spintronics, and solar-energy harvesting. In this particular study, we focus on a well-known 2D material, MoS_2, and show the emergence and spatial profile of these channels of free carriers at the edges of the nanoribbon.

Decomposition

The numerical simulation of the free-carrier density of a nanoribbon is decomposed into three main phases: pre-processing, density-functional-theory (DFT) simulations, and post-processing. Pre-processing involves the determination of the crystal structure of the nanoribbon by repeating the unit cell of the bulk crystal indefinitely along one direction and only a finite number of the times along another, together with the definition of a specific edge termination. DFT simulations are then required to fully relax the crystal structure of the nanoribbon by following the forces computed from first-principles and to determine the ground-state electronic density of the system. This has been obtained using the open-source suite of codes *Quantum ESPRESSO* (http://quantum-espresso.org). Finally, post-processing involves the extraction of the free-carrier density and its qualitative representation (visualization). The density of free electrons and holes has been obtained by integrating the local-density of states respectively over filled conduction-band states and emptied valence-band states, using an *ad-hoc* Fortran code specifically designed for this problem.

Visualization

In the visual representation we show the spatial profile of the charge density of free electrons (blue) and holes (red), obtained by selecting specific isosurfaces. The crystal structure is illustrated using a ball-and-stick representation, while a depth-cueing effect has been adopted to convey the sense of a nanoribbon infinitely extended away from the viewer. In front, the ribbon and the free-charge density have been cut to better reveal the crystal structure and the nature of the atomic orbitals involved in the channels. Scientifically, the selected image clearly indicates the emergence of one-dimensional wires of free electrons and free holes that are localized at opposite edges of a nanoribbon. The open-source software VMD (Visual Molecular Dynamics, http://www.ks.uiuc.edu/Research/vmd/) was used to create the image, which was then rendered using the Tachyon ray tracing system.