Engineering polar discontinuities in 2D honeycomb lattices

Marco Gibertini¹, Giovanni Pizzi¹, Nicola Marzari¹

¹) Theory and Simulation of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

Corresponding author: Marco Gibertini (marco.gibertini@epfl.ch)

Unprecedented and fascinating phenomena have been observed at oxide interfaces between centrosymmetric cubic materials, where polar discontinuities can give rise to polarization charges and electric fields that drive a metal-insulator transition and the appearance of a two-dimensional electron gas. Lower dimensional analogues are possible, with polar discontinuities and electron or hole wires emerging at interfaces in honeycomb lattices. Here we suggest different realistic pathways to engineer electronic and hole wires in 2D materials and devices, and support these suggestions with extensive first-principles calculations. Several approaches are discussed, based on: (i) nanoribbons, where a polar discontinuity against the vacuum emerges; (ii) functionalizations, where covalent ligands are used to introduce polar discontinuities by selective or total functionalization of the parent systems; and (iii) structural interfaces, including inversion domain boundaries and phase-engineered interfaces. All the cases considered have the potential to deliver innovative applications in ultra-thin and flexible solar-energy devices and in micro- and nano-electronics.