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One-dimensional metallic wires at phase-engineered boundaries in two-dimensional materials MARCO GIBERTINI, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne, Switzerland — At the interfaces between systems with different electric polarization, free carriers appear in order to screen the resulting polarization charges associated with the resulting polar discontinuity. This mechanism is believed to be at the origin of the two-dimensional electron gas emerging at oxide interfaces and provides the basis for manifold exciting novel phenomena. Recently, it has been shown that similar processes take place also in two-dimensional materials, where one-dimensional wires of free carriers are induced at planar interfaces between materials with different in-plane polarization or at the edges of polar nanoribbons. Here we show by first-principles simulations that some two-dimensional polar materials can display a metastable non-polar phase, so that boundaries between the stable and metastable phases support a polar discontinuity and the resulting one-dimensional metallic wires. We provide several approaches to engineer such phase boundaries by locally inducing metastable phases in a single parent crystal. We finally show how this novel strategy to engineer polar discontinuities in two dimensions offers unprecedented opportunities to efficiently manipulate and reconfigure the emerging one-dimensional metallic wires or switch their conducting state.

Marco Gibertini
EPFL, Switzerland

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