Engineering polar discontinuities in honeycomb lattices

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Unprecedented and fascinating phenomena have been recently 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, and honeycomb lattices offer a fertile playground thanks to their versatility and the extensive on-going experimental efforts in graphene and related materials. Here we suggest different realistic pathways to engineer polar discontinuities in honeycomb lattices, 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, and (ii) functionalizations, where covalent ligands are used to engineer polar discontinuities by selective or total functionalization of the parent systems. 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.