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Electronic structure of stacking faults in hexagonal graphite KLAUS KOEPERNIK, MANFRED TAUT, MANUEL RICHTER, IFW Dresden, Germany — We present results of self-consistent, full-potential electronic structure calculations for slabs of hexagonal graphite with stacking faults. There are two types of stacking faults, which differ qualitatively in their chemical bonding picture. We find, that both types induce localized interface bands near the symmetry line K-M in the Brillouin zone and a related peak in the local density of states (LDOS) very close to the Fermi energy, which should give rise to a dominating contribution of the interface bands to the local conductivity at the stacking faults. In contrast, a clean surface does not host any surface bands in the energy range of the π and σ bands, and the LDOS near the surface is even depleted. On the other hand, displacement of even one single surface layer induces a surface band near K-M. A special role play unsaturated monomer p_z-orbitals in the vicinity the stacking faults. The formation energy of both types of stacking faults and the surface energy are discussed.

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