Direct Determination of the Chemical Bonding of Individual Impurities in Graphene.

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Abstract

Using a combination of Z-contrast imaging and atomically resolved electron energy-loss spectroscopy on a scanning transmission electron microscope, we show that the chemical bonding of individual impurity atoms can be deduced experimentally. We find that when a Si atom is bonded with four atoms at a double-vacancy site in graphene, Si 3d orbitals contribute significantly to the bonding, resulting in a planar sp^2d-like hybridization, whereas threefold coordinated Si in graphene adopts the preferred sp^3 hybridization. The conclusions are confirmed by first-principles calculations as implemented in the Vienna Ab initio Simulation Package and demonstrate that chemical bonding of two-dimensional materials can now be explored at the single impurity level[1].

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