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Direct Determination of the Chemical Bonding of Individual Impurities in Graphene[1] MYRON KAPETANAKIS, WU ZHOU, MICAH PRANGE[2], SOKRATES PANTELIDES, Dept. of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, USA. MST Division, ORNL, Oak Ridge, TN 37831, USA, STEPHEN PENNYCOOK, MST Division, ORNL, Oak Ridge, TN 37831, USA. Dept. of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, USA, JUAN-CARLOS IDROBO, MST Division, ORNL, Oak Ridge, TN 37831, USA — 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 and demonstrate that [U+2028] chemical bonding of two-dimensional materials can now be explored an experimental probe at the single impurity level.

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[2]Present address: Pacific Northwest National Laboratory, Richland, WA 99352, USA.

Myron Kapetanakis
Dept. of Physics and Astronomy, Vanderbilt University,
Nashville, TN 37235, USA.
MST Division, ORNL, Oak Ridge, TN 37831, USA

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