Graphene on Ru(0001): contact formation and chemical reactivity on the atomic scale

S. J. Altenburg[1], J. Kröger[2], B. Wang[3], M.-L. Bocquet[3], N. Lorente[4] and R. Berndt[1]
[1]Institut für Experimentelle und Angewandte Physik,
Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany
[2]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany
[3]Université de Lyon, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon,
CNRS, F69007 Lyon, France
[4]Centre d'Investigació en Nanociència i Nanotecnologia (CSIC-ICN),
Campus de la UAB, E-08193 Bellaterra, Spain
altenburg@physik.uni-kiel.de

Graphene layers with a high degree of perfection may be grown on crystal surfaces, where the interaction with the substrate modifies its electronic properties to varying degrees. On most transition metals superstructures occur and lead to periodic modulations of geometric, electronic and bonding properties.
Here, we use a low-temperature scanning tunneling microscope (STM) to probe with atomic precision the conductance G = I / V (I: current, V : sample voltage) of junctions comprising a Au tip and a single graphene layer on Ru(0001). On this substrate graphene forms a hexagonal moiré superstructure with a periodicity of ≈ 30Å, which involves a buckling of the graphene sheet and a strongly inhomogeneous electronic structure. Our STM measurements directly probe the chemical reactivity of graphene during bond formation between tip and sample and reveal its location on the atomic scale. This is possible owing to significant variations of the tip-graphene contact formation process and of the conductance within the moiré unit cell. A smooth transition from tunneling to contact occurs in regions where the graphene layer is buckled away from the substrate, while in the strongly bound parts a jump to contact is observed, similar to point contacts on pristine noble metal surfaces. This behavior can be traced back to the different electronic structure and ultimately to the different chemical reactivity of the graphene layer as revealed by density functional theory. Variations in the conductance at contact formation within the moiré unit cell can be attributed to differing graphene-Ru-distances, as indicated by quantum transport calculations utilizing non-equilibrium Green's functions techniques.