Artificial two-dimensional Mott insulating superstructures with a large Mott gap

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Abstract:

Mott insulators, particularly those with a large Mott gap such as the transition metal oxides, are significant for the study of interplay between Mott physics, high-Tc superconductivity and quantum spin liquid. Efforts have been made to obtain a large-gapped Mott insulator through applying pressure, electric field and doping. However, most of the discovered Mott insulators host a much smaller gap than the transition metal oxides. Here, we report a method to realize the two-dimensional (2D) Mott insulating structures with a large Mott gap of a few electron volts. Instead of the transition metals with d orbital electrons, we adopted only Sn atoms with s and p orbital electrons to construct the artificial 2D atomic structures in large periodicity on the base of Sn/Si(111), i.e., , and . In this way, the electron orbitals are hybridized, and meanwhile the hopping is tuned effectively, leading to the large Mott gaps ranging from 2.5 eV to 3.1 eV, as corroborated by the theoretical model of xxx. The good consistence between experimental observations and theoretical proposal based on the Mott-Hubbard model suggests that these large-periodicity superstructures are 2D Mott insulators with prominently large Mott gaps. Our study offers a new possible platform for further study of strong correlation physics.

Introduction

Mott insulating state is induced by the strong electron correlation effect, and may give rise to other exotic states, such as unconventional high-Tc superconductivity (SC) and quantum spin liquid state (QSL), through spin frustration or electron doping [1](#_ENREF_1), [2](#_ENREF_2). The basic Mott physics can be well captured by the Hubbard model [3](#_ENREF_3). When the on-site repulsive Coulomb interaction (U) dominates over the kinetic energy (proportional to hopping integral, t), the electrons are prevented from doubly occupying a site and then are localized at each site. So there is an energy separation of U between electrons that occupied an empty site and a site already taken by another electron. As a result, the band is split into the lower and upper Hubbard bands and thus a Mott-Hubbard gap opens for a half-filling [4](#_ENREF_4). Driven by the interests on understanding the mechanism of unconventional superconductivity and searching for the candidate materials of QSL states, a number of Mott insulators have been discovered and extensively explored in the past few decades, including transition metal oxides (e.g., cuprates and Ir oxides[5-7](#_ENREF_5)), transition metal dichalcogenides (e.g., 1T-TaS2 and 1T-TaSe2[8-11](#_ENREF_8)), organic compounds[12-14](#_ENREF_12), C603- fulleride family[15](#_ENREF_15) and stacked graphene[16-18](#_ENREF_16).

The size of Mott gap is generally determined by the ratio of U/t. The transition metal oxides host a large Mott gap of ~ 2-3 eV, which is primarily attributed to the strong on-site Coulomb interactions of the 3d electrons (large U)[19](#_ENREF_19), [20](#_ENREF_20). For the materials with a moderate U that is not strong enough to directly open a Mott gap, e.g., 1T-TaS2, C603- fulleride family and stacked graphene, the expected distinct narrow bands (small t) at half-filling around EF is mainly responsible to the Mott transition, with a much smaller Mott gap of tens to hundreds of meV [17](#_ENREF_17), [21](#_ENREF_21), [22](#_ENREF_22).

As exemplified by the transition metal oxides, a Mott insulating state with a prominently large Mott gap can provide a valuable model for the study of interplay between Mott physics, high-Tc superconductivity and QSL. Various methods, such as applying pressure[23-27](#_ENREF_23), electrical field[18](#_ENREF_18) or chemical doping[28](#_ENREF_28), have been explored to tune the Mott insulating states through varying U and t. However, it turns out that to obtain a large-gapped Mott insulator is rather challenging. In addition, to construct artificial structures provides a more flexible way to intrinsically tune the electron correlation effects through tunable parameters such as the lattice symmetry and interatomic spacing [29](#_ENREF_29). These lattice variations can modulate the on-site Coulomb interaction and hopping integrals and therefore effectively modify the crucial parameter of U/t in Mott insulators.

Mott insulating ground state has been realized on the sub-monolayer of adsorbed atoms on (111) semiconductor substrates, e.g., K/Si(111)[30](#_ENREF_30) and Sn/Si(111)[31-33](#_ENREF_31), forming the desired artificial two-dimensional (2D) lattice. Here, we provide a new scenario to rearrange atoms and construct artificial lattices, on the base of Sn/Si(111)-. Three new ordered superstructures were subsequently obtained by annealing the as-deposited Sn/Si(111) surfaces, as determined as the , and respectively. *In-situ* STS measurements demonstrate the large insulating gaps of 2.5 eV, 3.1 eV and 2.95 eV respectively on these surfaces. The observed insulating gaps are uniform at different atom sites, in consistent with the theoretical proposal based on Mott-Hubbard model. It suggests that the three different ordered superstructures are Mott insulators with prominently large Mott gaps. The experimental realization of this artificial tunable Mott insulators with large Mott gaps offers a new platform for shedding light on Mott physics and provides possibility for further realizing high temperature SC or QSL states.

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