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Two Dimensional Triangular Lattice Mott-Hubbard Insulators in Real Life: Sn/Si(111), Sn/Ge(111) and other surfaces

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Genuinely two-dimensional (2D) Mott-Hubbard (MH)insulators are hard to come by in nature, although they should be interesting to work with. Semiconductor surface states form narrow half filled bands which have long been considered a natural place to look for strong electron correlations and 2D metal-insulator transitions including periodically distorted charge (and spin) density waves [1]. Surfaces isoelectronic to (1/3) coverage, (sqrt3 x sqrt3) periodic Sn/Si(111), Sn/Ge(111), Si/SiC(0001) are endowed precisely with such a narrow half filled band, and appear to provide an ideal playground [2, 3]. Among these, SiC(0001) has been known to possess an undistorted MH insulator ground state, whereas Sn/Ge(111) is a (3x3) periodically distorted metal, and Sn/Si(111) an undistorted (sqrt3 x sqrt3) metal[2,3]. While this diversity is in agreement with conventional local density functional (LDA) calculations, (where MH insulators do not exist or appear disguised as magnetic band insulators as in SiC(0001)) it is still surprising, in view of their extremely narrow half filled surface bands. The apparent diversity of behavior was recently removed by the experimental discovery that even Sn/Ge(111) and Sn/Si(111), contrary to LDA predictions, revert to undistorted MH insulators below 20 K and 60 K respectively [4, 5].

I will describe improved density functional LDA+U calculations which, while still mean field in character, enforce better the requirement of integer site occupancy. In Sn/Ge(111) at T=0, one finds that a distorted (3 x 3) metal and a (sqrt3 x sqrt3) undistorted insulator are both possible, the insulator prevailing for realistic U values. For Sn/Si(111), realistic values of U turn the ground state from a metal to a narrow gap insulator. These results naturally explain the emergence of MH ground states in agreement with experiment [6].

In these MH insulating surfaces it is predicted that each Sn adatom supports a spin 1/2. Spins on nearby adatoms interact antiferromagnetically through an exchange coupling J, in the range of 50 K for Sn/Ge(111), and 100 K for Sn/Si(111). Thus the Mott-Hubbard insulating ground state of these surfaces is a realization of the 2D triangular Heisenberg antiferromagnet. Below kT J the spins cannot fluctuate independently of one another, and in this regime spin entropy will be effectively frozen. This observation may explain the observed transition of Sn/Ge(111) and Sn/Si(111) from an undistorted low temperature MH state to a metallic band-like state at higher temperature [3, 4, 5]. The possible resonating valence bond (RVB) state of these insulating surfaces suggests that their doping through alkali adsorbtion or other means might lead to novel 2D d-wave (quasi) superconducting states.

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