Réunions scientifiques

Séminaires

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

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Invité par Amina TALEB

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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 give rise to narrow half filled bands, long regarded as a natural place to look for strong electron correlations and 2D metal-insulator transitions, including periodically distorted charge (and spin) density waves[1]. Semiconductor surfaces that are isoelectronic to (1/3) coverage, (sqrt3 x sqrt3) periodic Sn/Si(111), Sn/Ge(111), Si/SiC(0001) are all endowed with precisely such a narrow half filled band, and appear to provide the ideal playground for this problem.[2,3] Among these, only SiC(0001) is currently believed to possess an undistorted MH insulator ground state, whereas Sn/Ge(111) is metallic and displays a (3x3) periodic 2D lattice distortion, and Sn/Si(111) seems a simple undistorted (sqrt3 x sqrt3) metal[2,3]. While this diversity seems in agreement with conventional local density functional (LDA) calculations, where MH insulators either do not exist or appear (as in SiC(0001)) disguised as magnetic band insulators -- it is still surprising, in view of their extremely narrow half filled surface bands in all these systems.

This apparent diversity of behavior was recently removed by the experimental reports that even Sn/Ge(111) and Sn/Si(111), contrary to LDA predictions, revert to undistorted insulators, probably of MH nature, 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 the requirement of integer site occupancy to an extent controlled by the Coulomb repulsion parameter U. 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 a Mott-Hubbard insulating ground state on these surfaces would be 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 should be effectively frozen out. This observation may explain the observed transition, or crossover, 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 a 2D d-wave (quasi) superconducting state.

[1]. E. Tosatti and P. W. Anderson, Jap. J. Appl. Phys., Pt. 2, Suppl.2, 381 (1974); E. Tosatti, Festkoerperprobleme (Advances in Solid State Physics), Pergamon/Vieweg, Braunschweig, 15, 113 (1975).
[2] L. Petersen, Ismail, and E. W. Plummer, Prog. Surf. Sci. 71, 1 (2002)
[3] G. Santoro, et al., Phys. Rev.B 59, 1891 (1999)
[4] R. Cortes et al, Phys. Rev. Lett. 96, 126103 (2006)
[5] S. Modesti, et al., Phys. Rev. Lett. 98, 126401 (2007)
[6] G. Profeta and E. Tosatti, Phys. Rev. Lett. 98, 086401 (2007)

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