MAR10-2009-002724

Abstract for an Invited Paper
for the MAR10 Meeting of
the American Physical Society

Maximally anisotropic point Fermi surface system: VO_2 films embedded in TiO_2

VICTOR PARDO, Departamento de Fisica Aplicada, Universidade Santiago de Compostela, Santiago de Compostela, E-15782 Spain

Oxide heterostructures provide an unusually rich canvas for the design of unprecedented electronic states. Here we will discuss multilayer $(TiO_2)_m/(VO_2)_n$ nanostructures, namely V^{4+}:d^1 - Ti^{4+}:d^0 interfaces, with no polar discontinuity, studied by density functional theory techniques[1]. This system shows a metal-insulator transition with respect to the VO_2 layer thickness in our first principles calculations[2]. For n = 1 and 2 VO_2 layers, the system is insulating. For 5 and more layers, it is ferromagnetic and half-metallic. For the quantum confined cases of n = 3 and 4 the system is neither insulating nor conducting, instead an unexpected state arises: the Fermi surface is point-like as in graphene, except that extreme anisotropy is present[3]. The electrons (or holes, depending on doping) behave as massless fermions along the zone diagonal in k-space, and as conventional (massive) fermions along the perpendicular direction. Certain characteristics identify this "semi-Dirac" phase as resulting from quantum confinement, rather than being an interface phenomenon. This point Fermi surface system differs from graphene not only in its extreme anisotropy, but that it arises in a half-metallic system, so spin degrees of freedom are removed. In this presentation an analysis of the evolution of the electronic structure through this unprecedented insulator-to-metal transition will be provided, and the role of a non-intuitive orbital ordering of the V d^1 ions will be discussed. Also the robustness of the semi-Dirac electronic structure to interfacial disorder and the introduction of spin-orbit coupling in the calculations will be analyzed.

[1] V. Pardo and W.E. Pickett, Phys. Rev. Lett. 102, 107003 (2009).
[2] V. Pardo and W.E. Pickett, arXiv:0910.4411.
[3] S. Banerjee, R.R.P. Singh, V. Pardo and W.E. Pickett, Phys. Rev. Lett. 103, 016402 (2009).