Observation of non-adiabatic Kohn anomalies on Bi(111) - Inducing spin-flip electronic transitions using helium Atom Scattering

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The unique property of Bismuth showing metallic behavior at the surfaces but semimetallic and even insulating behavior in the bulk promise applications using nano-scale structures. This surface specific metallic behavior is caused by the strong spin-orbit splitting present in bismuth. Earlier assumptions of the formation of a charge-density wave on the Bi(111) surface [1] were discarded, since the nesting vectors touching the Fermi surface at $k_F = 0.0532 \mp 0.0003$ Å^{-1} and $-k_F$ respectively, as suggested in [1] are spin-opposing states, as predetermined by time-reversal symmetry [2]. Recent inelastic Helium Atom Scattering (iHAS) experiments revealed strongly pronounced narrow dips in the phonon dispersion relation of the Bi(111) surface. The position of these dips indicates a Kohn-like anomalous interaction with the very same nesting vector as Ast and Höchst suggested. Such an anomaly is only possible considering the coupling of non-adiabatic electronic transitions to the lattice vibrational movements. Recently a very similar situation was found on the surface of the topological insulator Bi2Se3 [3], where the spin disparity between k_F and $-k_F$ given by time-reversal symmetry yields the striking properties of this materials class to “prohibit electronic U-turns” [4]. Those non-adiabatic Kohn anomalies provide a fundamental difference between iHAS measurements and theoretically predicted surface phonon energies, since non-adiabatic effects are not accessible using standard DFPT-methods.

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[2] T. K. Kim et. al, PRB 72, 085440, 2005

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[4] M. Franz, Nature 466, 323, 2010