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Session R43: Electron Transfer, Charge Transfer and Transport

2:30 PM–5:30 PM, Wednesday, March 20, 2013 Hilton Baltimore Room: Holiday Ballroom 2

Sponsoring Unit: DCP

Abstract: R43.00003 : Possibilities for Observation of Quantum Transport in (RE)Ba\$_{2}\$Cu\$_{3}\$O\$_{\mathrm{7-y}}\$ Perovskites 2:54 PM-3:06 PM

Preview Abstract

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For y \$\approx \$ 0, the crystal structure of the ``1-2-3" family of rare earth copper oxide perovskites displays several curious ``porosity" features. For example, along the b-axis direction of the region usually termed the ``CuO chains," one observes a dramatically wide ``channel" bounded within a Ba-Cu-O tube. Similar channels can be found in both the b- and a-axes directions contained within RE, Cu and O ion groupings. The cross-sectional area of these channels is roughly that of a single-wall carbon nanotube, suggesting the former may manifest Buettiker-Landauer quantum conductance similar to that observed in the latter. Moreover, by employing various ratios of Pr/Y for the RE component of the host system, the bulk electrical properties of the surrounding host can be tailored from completely insulating to metallic. We test our conjecture predicting ballistic transport down these channels using density functional theory and report our initial findings here along with the likely consequences of paramagnetic spin scattering. We also discuss possible experimental embodiments which could lead to nano-controllable gate structures.

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