SESSION VV4: The Mechanism for high-Tc and the Quest for New Superconductors
Chair: Claudia Cantoni
Wednesday Morning, April 27, 2011
Room 2020 (Moscone West)

9:00 AM VV4.2

A DFT (LDA+U) Study of the Electronic Properties of Square-planar Coordinated Copper Monoxide Structures. Paul M. Grant, W2AGZ Technologies, San Jose, California.

It is now 25 years and three months since Georg Bednorz observed the onset of high temperature superconductivity in copper oxide perovskites, and yet its origin remains still largely unresolved. However, it quickly became evident the phenomenon was restricted to those structures possessing a common feature -- square planar coordinated "sheets," or "layers" of copper monoxide, now believed essential to the existence of superconductivity in these materials. We examine the structural stability and electronic properties of both “sheets” and “tubes” of CuO in such coordination as a function of Hubbard U within the DFT (LDA+U) framework , and for those values which yield metallic band structures, their fermiology and hole/electron-phonon coupling, and where applicable, Landauer-Buettiker ballistic transfer. Although such compounds do not, as yet, exist, we consider their study via DFT as proxies to aid eventual general understanding of superconductivity in layered copper oxide perovskites.