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A DFT (LDA+U) study of the electronic properties of layered, square-planar coordinated, copper monoxide structures PAUL M. GRANT, IBM Research Staff Member Emeritus, San Jose, CA 95120 USA — It is now 25 years and two months since Georg Bednorz observed the onset of high temperature superconductivity in copper oxide perovskites, and yet today 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, and thus now thought to be essential to effect superconductivity in this family of materials. We examine the structural stability and electronic properties of these 2D approximations to the layered CuO compounds as a function of Hubbard U within the DFT (LDA+U) framework, especially for those particular values yielding metallic band formation, and their subsequent fermiology and electron/hole-phonon coupling properties. Although such particular 2D embodiments do not, as yet, exist, we consider their study via DFT as valuable proxies[1] to aid eventual understanding of that flavor of superconductivity revealed by the Bednorz-Mueller breakthrough.

[1]P. M. Grant, Journal of Physics: Conference Series **129** (2008) 012042.

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