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Properties of extended inorganic solids predicted/rationalized by First Principles electronic structure calculations

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Due to the vastly complex nature of the problem, guidelines for the preparation of extended inorganic solids with specific electronic properties remain meagre. Here we present the use of First Principles LMTO band structure calculations for the rationalization of the properties of a number of interesting extended solids. These include metallic or semiconducting behaviour in some delafossite oxides [1] and the paraelectric to antiferroelectronic transition in an elpasolite associated with the localization of the lone pair on Pb [2]. Through an analysis of the electronic structures of a number of superconductors [3–5], we find certain crucial features that permit us to propose candidate systems that might display this phenomenon. Through a related analysis of magnetic systems (isostructural with the superconductors) using spin-polarised calculations [3,6], we rationalize and predict the phenomenon of giant (or colossal) magnetoresistance (GMR) in a number of compounds. Some of these predictions have already borne fruit [7].

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