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Fate of magnetic-electronic properties of transition-metal compounds at extreme conditions

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During the past two decades insulating 3d transition-metal (TM) compounds became the focus of intensive basic and applied research in materials science. The main reason was the important discoveries of high-TC superconductivity in doped rare-earth copper-oxides (e.g., La₂CuO₄), and recently in the layered iron arsenic compounds (e.g., BaFe₂As₂), the observation of giant magneto-resistance effects in doped manganese oxides (La_{1-x}Ca_xMnO₃) and more recently multiferroic behavior (e.g., BiFeO₃ and TbMnO₃) where there is coexistence of more than one ferroic order, e.g., coupling between magnetism and ferroelectricity. Currently 4d and 5d TM systems (e.g., Sr₂RuO₄ and Na₂IrO₃) are in vogue.

The intrigue surrounding these compounds is that they have partially filled d-bands and in terms of conventional Bloch-Wilson band theory, they should then be metallic. Yet the majority of these compounds are insulating! Many have large optically probed band gaps of eV magnitude, and the ground state is antiferromagnetic. Mott's effort in the nineteen-fifties and subsequent research in the next decade lead to the recognition that <u>on-site</u> (intra-atomic) Coulomb repulsion of electrons in comparison with their hopping capability, manifested in the 3d bandwidth derived from inter-atomic overlap integrals, renders the insulating behavior. When the on-site repulsion is dominant, this is the regime of strongly correlated electrons (like "motor car traffic on the highway"). These so-called Mott insulators signify a breakdown of the independent quasi-particle approximation adopted in conventional band theory. Many deep Earth geophysical materials also fall into this category.

There has since been intense scrutiny of these systems up to date. The pertinent on-site Coulomb repulsion, referred to as the Hubbard U , results in a splitting of the 3d band into a lower Hubbard (valence) and upper Hubbard (conduction) band. Details of the 3d electronic band structure are important to describe both the physical properties and tunability of these properties to suit various applications. These details include relevant energy scales like : 3d bandwidth W, on-site repulsion U, intra-atomic d–d exchange energy (Hund's spin proximity rule) J, crystal-field splitting Delta;_{CF} and charge transfer energy Delta;_{CF} (cost of transferring charge from an anion neighbor to the TM cation).

Both the bandwidth W and Delta;_{CF} are particularly susceptible to tuning by varying the inter-atomic spacing by means of applied pressure. Consequently pertinent ratios like U/W and Delta;_{CF} / J can be varied over large ranges, with profound effects on the physical properties of the material. For example, correlation breakdown and an associated insulator -> metal transition may ensue (so-called Mott transition). Alternatively Hund's rule may breakdown and spin-pairing (re-distribution of electrons in the d-orbitals) may occur. These have significant implications for the magnetic properties at reduced inter-atomic spacings. How are these effects investigated experimentally?

Electronic/magnetic transitions in strongly correlated TM compounds, particularly Fe-based compounds in this “new iron age”, in a regime of very high static density are therefore the main consideration in this presentation. The focus will be on the above-mentioned topics and state-of-the-art experimental high pressure studies: employing diamond anvil cells (DACs) capable of generating static pressures beyond 100 GPa (a million atmospheres) and suitable experimental probes of electronic/magnetic properties of microscopic samples under these stringent extreme conditions. These include, (i) synchrotron x-ray based probes of magnetic-electronic behavior and (ii) complementary conventional ⁵⁷Fe Mössbauer effect spectroscopy, a premier magnetic probe for Fe-containing compounds. These need to be considered in conjunction with other techniques like (iii) electrical resistance R(P,T) and (iv) x-ray diffraction techniques, to establish the interplay between magnetic-electronic properties and both the electrical-transport and structural response of the systems of interest.

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