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Magnetic-electronic studies at a megabar: the new frontier

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The main consideration in this presentation is the interplay amongst magnetic-electronic, structural and charge-gap responses in strongly correlated 3d electron systems (transition metal oxides) evolved to very high static densities. Tuning through the large, ~eV, energy scales necessitate employing diamond anvil cells for requisite static pressures to the vicinity of ~100 GPa.
Consequently pertinent onsite-repulsion to bandwidth U/W and crystal-field splitting to spin-pairing energy CF/J ratios can be varied over large ranges. Profound effects on physical properties may ensue, including the breakdown of Hund's rule resulting in a high-spin (HS) to low-spin (LS) transition (CF/J > 1) and a Mott insulator-metal transition (U/W <1).
Variable temperature 57-Fe nuclear resonance (Mössbauer) spectroscopy extended to cryogenic temperatures, is one of the few and most powerful means of revealing the magnetic-electronic ground-state stabilized at high densities. Synchrotron XRD monitoring of the pressure evolution of the unit-cell volume provides evidence of crystallographic phase transitions or corroborating evidence of HS to LS transitions, from signature shrinkage effects in the cation radius due to spin pairing in lower lying 3d orbitals.
Complementary resistance pressure measurements help to ascertain whether magnetic collapse is associated with HS to LS crossover or correlation gap closure (insulator to metal transition) or the concurrence of the two phenomena.
Highlights from a selection of studies, which include synchrotron XRD and nuclear resonance probes, on various ferrous spinels pressurized to the vicinity of ~100 GPa will be presented [1-3]. These include, as a result of compression: (i) orbital moment quenching effects, (ii) site-inversion at room temperature and subsequent spin crossover occurring, (iii) transitions to post-spinel structures and subsequent triggering of partial/site-specific spin crossover, (iv) charge-gap resilience in spite of anticipated appreciable bandwidth broadening and an attempt to rationalize this.
We will further indicate why probing magnetic-electronic and structural aspects of these transition metal oxides beyond ~100 GPa would be useful, is beyond home laboratory based capabilities and that synchrotron probing with appropriately tightly focused probes of micron or sub-micron dimensions is imperative.

References

[1] W. M. Xu, G. R. Hearne, S. Layek, et al., Phys. Rev. B 95, 045110 (2017).
[2] W. M. Xu, G. R. Hearne, S. Layek, , et al., Phys. Rev. B 96, 045108 (2017).
[3] W. M. Xu, G. R. Hearne, S. Layek, et al., Phys. Rev. B 97, 085120 (2018).

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