Oral Contributions

[MS20] Crystal physics of minerals and materials at variable pressures and temperatures

Co-Chairs: Anna Gagor (PL); Vitali Prakapenka (US)

[MS20-01] Structural consequences of pressure-induced electronic transitions in iron compounds*

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Electronic/magnetic transitions and their structural consequences in Fe-based Mott insulators in a regime of very high static density are the main issue of this lecture. The lecture is based primarily on our previous and ongoing experimental high pressure studies employing: (*i*) diamond anvil cells, (*ii*) synchrotron X-ray diffraction, (*iii*)^{57}Fe Mössbauer spectroscopy, (*iv*) electrical resistance and
(*v*) X-ray absorption spectroscopy. It is shown that applying pressure to such strongly correlated systems leads to a number of changes; including quenching of the orbital moment, spin crossover, inter-valence charge transfer, insulator–metal transition, moment collapse and volume collapse. These changes may occur simultaneously or sequentially over a range of pressures. Any of these may be accompanied by or be a consequence of a structural phase transition; namely, a change in crystal symmetry. Analyzing this rich variety of phenomena we show the main scenarios which such strongly correlated systems may undergo on the way to a correlation breakdown (Mott transition) and what are the structural consequences of these electronic/magnetic transformations. To illustrate these scenarios we present recent results for MFeO$_3$ (M = Fe, Ga, Lu, Eu, Pr) and CaFe$_2$O$_4$ ferric oxides; FeCl$_2$ and FeI$_2$ ferrous halides, and FeCr$_2$S$_4$ sulfide. Fe$_3$O$_4$ and Fe$_2$O$_3$ are given as example cases where Mössbauer Spectroscopy has improved the understanding of the data obtained with X-ray diffraction studies.

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Keywords: High pressure; crystallographic transition; magnetic/electronic transitions.