MS15-P03 | PRESSURE-INDUCED SPIN TRANSITIONS IN GARNETS

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Garnets are of high mineralogical interest as they belong to the most common minerals in the Earth's upper mantle. And garnet crystals are used in many types of applications, for example as scintillator cystals, phosphor materials, magnetic storage materials, laser crystals, and lithium batteries.

Here, we present a comparative study of the effect of cation and anion substitution in garnets on pressure-induced electronic (spin-pairing) transitions of 3*d*-transition-metal cations, i.e. Fe^{3+} and Mn^{3+}. The structural compression and spin transitions of OH-free manganese garnets $Ca_3Mn_2[SiO_4]_3$ and blythite, $Mn_3Mn_2[SiO_4]_3$ have been studied using single-crystal synchrotron X-ray diffraction at PETRA III, Raman spectroscopy, and theoretical calculations based on density functional theory at pressures of up to 75 GPa. Our new results will be compared with our recent results on andradite, $Ca_3Fe_2[SiO_4]_3$ and tetragonal henritermierite, $Ca_3Mn_2[SiO_4]_2[O_4H_4]$ [1,2], and with literature data on other Fe^{3+}-bearing garnets.

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[1] A. Friedrich et al., Phys. Rev. B **2014**, 90, 094105
[2] A. Friedrich et al., Phys. Rev. B **2015**, 92, 014117