MS36-P1 **Crystal Chemistry of Fe,Al-bearing Silicate Perovskites at High Pressures and Temperatures.** Leonid Dubrovinsky,[a] Konstantin Glazyrin,[a] Tiziana Boffa-Ballaran,[a] Elena Bykova,[a] Marco Merlini, [b c] Michael Hanfland,[c] Natalia Dubrovinskaia[d] *[a]Bayerisches Geoinstitut, Universität Bayreuth, Germany, Country, [b]Dipartimento di Scienze della Terra, Universitŕ degli Studi di Milano, Italy, [c]ESRF, Boîte Postale 220, 38043 Grenoble, France, [d]Lehrstuhl für Kristallographie, Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth, Germany*
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Modern science and technology rely on the fundamental knowledge of matter that is provided by crystallographic studies. The most reliable information about crystal structures and their response to changes in pressure and temperature is obtained from single crystal diffraction experiments. Advantages in diamond anvil cell techniques (DACs) and modern X-ray sources have increased the accessible pressure range for structural research up to several dozens gigapascals. We have develop a methodology to perform single crystal X-ray diffraction experiments in double-side laser-heated DACs and demonstrate that solution of crystals structure refinements and accurate measurements of the thermal equation of state of metals, oxides, silicates from single crystal intensity data are possible in a megabar pressure range at temperatures of thousands degrees. Particular attention we paid on in situ study of geomaterials at extreme conditions. We studied silicate perovskites (Mg0.88Fe0.12)SiO3, (Mg0.9Fe0.1)(Si0.975Al0.025)O3, and (Mg0.6Fe0.4)(Si0.655Al0.35)O3, by means of single crystal X-ray diffraction in laser-heated diamond anvil cells, Mossbauer spectroscopy, and nuclear forward scattering at pressure up to 140 GPa and temperature above 2500 K. We will discuss effects of changes in iron electronic state on structure and properties of the materials.

Keywords: crystal chemistry, silicate perovskite, high pressure and temperature

MS36-P2 **Theoretical Probe on Effect of High Pressure on Thermophysical Properties of Perovskite Rare Earth Manganites.** Archana S. Srivastava,[a] N.K. Gaur,[b] *[a] Sri Sathya Sai College for Women, India, [b]Superconductivity Lab., Barkatullah University, India*
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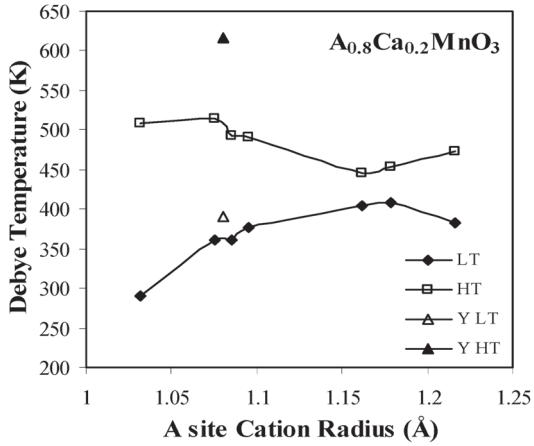
The doped perovskite $R_{1-x}A_xMnO_3$ (R=La, Pr, Nd, …Dy; A=Sr, Ca,…), are the interesting class of materials which exhibit Colossal Magnetoresistance (CMR), charge ordering and other multiferroic properties. [1]. We can control charge transport in these materials by externally controllable parameters like pressure, temperature and magnetic field and this makes them attractive as sensor material. However the studies regarding the effect of pressure on the thermophysical properties have not been initiated by many researchers whereas it is important to know the effect of increasing pressure above ambient conditions on charge transport and heat conduction of these materials. In the present investigation we will use the MRIM model and AIM theory to systematically probe the thermophysical properties of these complex inorganic compounds and study the effect of increasing pressure on these properties using an atomistic approach [2]. Present results conclude that specific heat is found to be dependent on the chemical pressure and it increases with the decrease of A-site cation radius or increase in external pressure. Also, this work reports, probably for the first time the relation of pressure to the lattice specific heat ($C_{p(lattice)}$) along with other properties like bulk modulus (B) using AIM theory, molecular force constant (f), Reststrahlen frequency (ν_0), Debye temperature (θ_D) and Grüneisen parameter of these manganites. The figure given here presents the variation of Debye temperature against chemical pressure.



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Keywords: complex inorganic compounds; specific heat; Debye temperature; perovskite oxides; structural analysis