conference abstracts

s11.m2.o3 **First principles elasticity of major silicate and oxide phases of the lower mantle and geophysical implications.** B.B. Karki. *Department of Chemical Engineering and Materials Science, Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN 55455, USA*

Keywords: mineralogical crystallography, theoretical studies of minerals, properties of minerals.

Detailed knowledge of elastic properties of relevant minerals at the pressure-temperature conditions of geophysical magnitudesprovides a fundamental basis to extract information on properties and processes of the Earth interior from the rich seismological database. However, the challenge of measuring the elastic constants at such conditions by means of experiment is still enormous. Over the past few years, first-principles approach within the framework of density functional theory has taken on an increased significance in exploring the elastic behavior of minerals including those relevant to the lower mantle - the largest single region of the Earth's interior. The remarkably high accuracy with which these parameter-free calculations have been able to reproduce the experimental observations, even of subtle features such as the elastic anisotropy, has prompted first-principles theory as an ideal compliment to experiment. I discuss the predicted high pressure elasticity of the major silicate perovskites and oxides of the lower mantle[1] and also recent results on their thermoelastic properties[2]. The study shows that the effects of pressure are predominant in the deep interior as pressure generally suppresses the temperature dependence. I present a quick analysis of the impact and implication of these theoretical results in interpreting the seismological observations[3]. This includes comparing the predicted P and S wave velocities with spherically averaged radial seismic profiles; relating the anisotropy due to preferred orientations of component minerals with the seismic anisotropy; and anticipating on thermal origin of the tomographically observed seismic velocity variations.

s11.m2.o4 **Electronic structure and electric field gradient calculations of Al_2SiO_5 polymorphs**. P. Blaha[1], M. Iglesias[2], K. Schwarz[1] and D. Baldomir[2], *[1] Inst.of Physical and Theoretical Chemistry, Vienna University of Technology, A-1060 Vienna, Austria, [2] Fisica Aplicada, Universidade de Santiago de Compostela, 15706 Santiago de Compostela, Spain.*

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We have studied the electronic structure of the three polymorphs of Al_2SiO_5, andalusite, sillimanite and kyanite by full-potential linearized-augmented-plane-wave (LAPW) calculations using the WIEN code[1]. These calculations are based on density functional theory and employ Perdew´s generalized gradient approximation (GGA)[2].

Total energy calculations verify in agreement with experiment, that andalusite is the most stable phase followed by sillimanite and kyanite.

We determined the electronic charge density distributions and find negatively charged oxygen ions with strong polarization effects. We could identify the role of Al or Si neighbors and their respective distances from oxygen and found that oxygen charge is depleted towards the short O-Si bonds, but enhanced in the directions of long O-Al bonds. The chemical bonding is not purely ionic in nature but has important covalent contributions.

Using the total electron density, the electric field gradients (EFGs) are calculated without further approximations[3] (no point charge model, no Sternheimer factors) and agree well (within 10 %) with available experimental data on Al[4]. Predictions for the EFG at all oxygen sites are also made. We identify the polarization of the valence p states (e.g. Al-3p) which results in slightly different occupation of p_x, p_y and p_z orbitals as the main source of the EFG, while core polarization (e.g. Al-2p) contribute at most 25 % to the total EFG. Since the EFG is related to this anisotropy of the charge distribution we could also demonstrate the relation between calculated (or measured) EFGs and nearest neighbor coordination and distances.

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