

icosahedra. The best estimate on the number of atoms in the unit-cell is not even an integer number, 320.1, originating from the introduction of partial occupancy of atomic sites in the X-ray structural analysis [1].

This work is the first attempt, using *ab initio* molecular dynamics, to study the stable configuration of the partially occupied sites (POS) in β -boron and to investigate POS impact on the electronic structure. We have found that the correlated POS configurations not only lower the total energy of the solid, but also widen the electronic band gap, giving consistent results with experiments.

The high pressure phases of boron[2,3] have also been studied with *ab initio* simulated annealing methods. We found that at around 120GPa, β -rhombohedral boron undergoes amorphization and that its electronic conductivity rises, due to delocalization of the electronics states near the Fermi level, consistent with experimental observations[2,3].

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[1] Slack G. A., et al., *J. Solid State Chem.*, 1988, **76**, 52. [2] Eremets M. I., et al., *Science*, 2001, **293**, 272. [3] Sanz D. N., et al., *Phys. Rev. Lett.* 2002, **89**, 245501.

Keywords: *ab initio* structural determination, high pressure structure, electronic structure

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Oxides Under Pressure: from Densified Silica to the Rheology of the Earth's Mantle

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The paper will describe recent advances in the atomistic simulation of oxides at extreme conditions of pressure. The simulations are carried out using interatomic force fields optimized by best fit on first-principles (density-functional theory) calculations. The paper will focus on two applications of the method: (a) the mechanisms of permanent densification in silica glass, and (b) the properties of dislocations in MgO, the second most abundant mineral in the Earth's lower mantle.

Keywords: simulation, DFT, high pressure

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Novel High-pressure Phases: Theory and Experiment

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Searching for new materials and new crystal structures at high pressures and temperatures is important for fundamental physics, for material sciences, and for understanding the structure and properties of planetary interiors. State-of-the-art computer simulations can fruitfully complement or even guide experimental efforts in this direction. Here, we present recent joint theoretical/experimental discoveries of new geophysically important phases of MgSiO₃ [1-3] and Al₂O₃ [4] with implications for the structure, dynamics, electrical conductivity, rheology and seismic signatures of the Earth's lowermost mantle.

[1] Oganov A.R., Ono S., *Nature*, 2004, **430**, 445. [2] Murakami M., et al., *Science*, 2004, **304**, 855. [3] Oganov A.R., Martonak R., Laio A., Raiteri P., Parrinello M., 2005, *in preparation*. [4] Oganov A.R., Ono S., *Proc. Natl. Acad. Sci.*, 2005, *submitted*.

Keywords: high pressure, *ab initio*, Earth's mantle

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MgSiO₃ Post-perovskite at D" Conditions

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The thermoelastic properties of the newly found post-perovskite polymorph of MgSiO₃, more stable than the Pbnm-perovskite phase at conditions close to those expected in Earth's D" region, has been investigated by first-principles and contrasted with those of the perovskite phase. We predict the major seismic trends such as velocity discontinuities, ratios of velocities and density anomalies, and anisotropy in aggregates with preferred orientation that should occur in the presence of this phase change. Consequences of this model mineralogy for the D" region will be discussed.

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Keywords: phase transition, mantle mineralogy, thermoelasticity

MS41 COMPUTATIONAL SOLUTIONS FOR HIGH-THROUGHPUT CRYSTALLOGRAPHY

Chairpersons: Duncan E. McRee, James Holton

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Crank - New Methods in Automated Structure Solution

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We present Crank[1], a suite to help a user perform automated macromolecular structure solution. In this aim, it uses novel programs, including CRUNCH2 for substructure determination and BP3 for substructure refinement and phasing. In addition, Crank uses other commonly used crystallographic programs including SOLOMON, DM and various programs within the CCP4 suite. Crank uses the CCP4i package for its user interface, this allows for tight integration into the CCP4 suite and presents the user with a familiar interface. Crank uses the XML eXtensible Markup Language to store, manipulate and compare data, this XML can subsequently be used to assist in data deposition. We have tested Crank on a large number of datasets, including datasets from the Joint Center for Structural Genomics, our results show that Crank often outperforms existing automated substructure solution packages, and can lead to solutions where existing methods fail. For more information, please visit the Crank web site: <http://www.bfsc.leidenuniv.nl/software/crank>.

[1] Ness S. R., de Graaff R.A.G., Abrahams J. P., Pannu N.S., *Structure*, **12**, 1753-1761.

Keywords: automated macromolecular structure solution, BP3, crunch2

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Parallel Data Processing for High Throughput X-ray Structure Determination

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The Structure Determination Core (SDC) of the Joint Center for the Structural Genomics (JCSG) has implemented a prototype system, Xsolve, which automates all of the processing steps needed to create an initial set of molecular coordinates from a dataset of diffraction images. The goal of Xsolve is to provide standardized, high quality data processing and automate the numerous time-consuming steps in the structure determination process. The current prototype produces a model that is over 95% complete in more than 80 % of the MAD cases