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***Ab initio* Simulations of Lattice Stability: An Effect of External Conditions.** Igor Abrikosov. *Department of Physics, Chemistry and Biology, Linköping University, Sweden.*
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Ab initio electronic structure theory is known as a useful tool for prediction of materials properties and for their understanding. However, majority of simulations still deal with calculations of total energies at zero temperature. In this talk we show that for large number of problems it is necessary to take proper experimental conditions into account to obtain reliable theoretical results. In particular, we show that the problem of lattice stability, the energy difference between different crystal structures of a material, can be consistently described by theory and experiment if the former is done at elevated rather than at zero temperature [1]. A decisive role of lattice vibrations will be illustrated by theoretical search for metastable fcc-related Si-N phases [2], which are the tissue phases of (Ti-Si)N thin film nanocomposites, as well as in first-principles study of stability of newly synthesized ternary perovskite Sc_3AlN and a family of its isoelectronic compounds Sc_3EN (E=B, Ga, In) [3].

[1] Asker C., Belonoshko A. B., Mikhaylushkin A. S., Abrikosov I. A., *Phys. Rev. B,* **2008**, 77, 220102(R). [2] Alling B., Isaev E. I., Flink A., Hultman L., Abrikosov I. A., *Phys. Rev. B*, **2008**, 78, 132103. [3] Mikhaylushkin A. S., Höglund C., Birch J., Czigány Zs., Hultman L., Simak S. I., Alling B., Tasnady F., Abrikosov I. A., "Stability of ternary perovskites Sc_3EN (E=B, Al, Ga): first-principles theory", *Phys. Rev. B* (accepted, **2009**).

Keywords: ab-initio calculations; crystal structures; lattice dynamics

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Resonant X-ray Diffraction Distinguishes Inequivalent Iron Atoms in Fe_3BO_6. V. E. Dmitrienko[a], G. Beutier[b], E. N. Ovchinnikova[c], S. P. Collins[b], J. E. Lorenzo[d], J.-L. Hodeau[d], A. Kirfel[e], Y. Joly[d], A. A. Antonenko[c], V. A. Sarkisyan[a,f], A. Bombardi[b]. [a]*Institute of Crystallography, 119333, Moscow, Russia.* [b]*Diamond Light Source, Harwell Science & Innovation Campus, OX11 0DE, United Kingdom.* [c]*Physical Department of Moscow State University, 119899 Moscow, Russia.* [d]*Institut Louis Néel, CNRS, F-38042 Grenoble, France.* [e]*Steinmann Institute, University of Bonn, Poppelsdorfer Schloss, D-53115 Bonn, Germany.* [f]*Beam Engineering for Advanced Measurements Co., 809 South Orlando Ave., Suite I, Winter Park, FL 32789, USA.*
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It is demonstrated that, contrary to XANES and EXAFS, resonant X-ray diffraction can successfully distinguish atoms of the same element occupying inequivalent sites in the crystal structure. Forbidden Bragg reflections of iron orthoborate Fe_3BO_6 were studied theoretically and experimentally in the vicinity the iron *K*-edge. Their energy spectra are explained as resulting from the interference of X-rays scattered at two non-equivalent crystallographic sites occupied by the iron atoms. This particular structure property gives rise to complex energy and azimuthal dependences of the reflection intensities in the pre-edge region as they result from the interplay of site specific dipole-quadrupole and quadrupole-quadrupole resonant scattering. The interference is mainly constructive for the 300, 500 and 710 reflections, whereas the opposite holds for the 700 reflection. Best fitting of the main features of the intensity profiles was achieved by using different parameters for the excited states of the inequivalent iron atoms in the FDMNES code. Also evidenced is an anisotropic character of the absorption spectrum. Possible contributions of thermal vibrations and magnetic order are discussed. Particular care is given to extracting clean spectra from the data, and it is demonstrated that excellent results can be obtained even from measurements that appear corrupted by several effects such as poor crystal quality and multiple scattering.
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Keywords: resonant diffraction; forbidden reflections; iron orthoborate

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Pressure-Induced Phase Separation in High T_c Superconductors. Maria Calamiotou[a], Anestis Gantis[a], Dimitrios Lampakis[b], Eirini Siranidi[b], Kazimierz Conder[c], Irene Margiolaki[d], Efthymios Liarokapis[b]. [a]*Solid State Physics Dept., University of Athens, Greece.* [b]*Physics Dept., National Technical University, Athens, Greece.* [c] *Paul Scherrer Institute, Villigen, Switzerland.* [d]*ESRF, Grenoble, France.*
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It is now well accepted that structural and electronic inhomogeneities constitute intrinsic properties of cuprate superconductors. To this context the study of pressure-induced phase separation effects can improve our understanding on the role of lattice effects in the high T_c superconductivity. We present here the results of high pressure (up to 13GPa) synchrotron angle-dispersive powder diffraction experiments in comparison with high pressure micro-Raman data on different high T_c superconductors. 2D high quality diffraction images have been collected under high pressure using a diamond anvil cell (DAC) and a MAR345 image plate at the SNBL-BM01A beamline at ESRF. The c-axis of the optimally doped $YBa_2Cu_3O_y$ (Y123) cuprate exhibits in the pressure range 3.7GPa<p<10GPa a clear deviation from the expected equation of state while upon pressure release the data follow the anticipated dependence showing a strong hysteresis. At the pressure of ~3.7GPa new peaks appear in the diffraction pattern, which has being attributed to another apparently coherent phase that exhibits disorder and texture effects. Interatomic distances in the unit cell of Y123, such as the Ba distance from the basal plane, the Cu2-O_{pl} bond length and