Report by Alberto Garcia of his attendance to the Fall Meeting of the American Geophysical Union in San Francisco, December 10-14, 2007

I was invited to give a talk on the uses of the Siesta code in mineral physics. Siesta (see http://www.uam.es/siesta) is a computer program based on Density Functional Theory that, due to its efficiency and versatility, is increasingly being used by a wide variety of researchers in earth sciences.

Abstract for the talk
(The full presentation is being sent separately)

Applications of Efficient First-Principles Methods in Mineral Sciences: the SIESTA Program

The possibility of treating large systems with first-principles electronic-structure methods has opened up new opportunities in many disciplines. In particular, the SIESTA program (www.uam.es/siesta) has become quite popular and is increasingly being used by researchers in geosciences and biophysics. The code's efficiency for large problems stems from the use of strictly localized basis sets and from the implementation of linear-scaling algorithms which can be applied to suitable systems. A very important feature of the program is that its accuracy and cost can be tuned in a wide range, from very fast exploratory calculations to highly accurate simulations matching the quality of other approaches, such as plane-wave and all-electron methods. Even at the lower end of the range it provides a fully self-consistent solution that is more accurate than empirical approaches in problems involving charge transfer or coordination changes.

Apart from computing the electronic structure (including the effects of spin), the program can perform a full range of molecular dynamics simulations (including constant-stress) and structural optimizations, making it suitable for a wide spectrum of research topics in mineral sciences, some of which will be highlighted in the talk.

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Highlights of the meeting

The AGU meeting is quite large (an estimated 15000 people attended this edition), and I concentrated my attention mainly in the series of symposia organized by the division of Mineral and Rock Physics, consisting of oral presentation sessions, and poster sessions:

Multidisciplinary Approaches to the Study of Planetary Ices
Advances in Computational Studies of Earth Materials
Melts in the Deep Interior of the Earth
Structure and Properties of Silicate Melts
Diffusion, Defects, and Transport Properties in Geomaterials
Quantification of Rock Fabrics
Behavior of Iron in the Deep Earth and New Views of the Mantle and Core
Frontiers in the Chemistry and Physics of the Earth's Mantle Rock Physics
Plasticity of Minerals at High Pressures and Temperatures and Implications for Deep-Earth Rheology and Anisotropy
Shock Metamorphism and Mineral Physics of Dynamic Compression
Structures and Properties of Earth's Interior Probed Using Advanced Radiation, Laboratory Tools, and Seismic Waves

The most noteworthy developments in my opinion were:

* The variety of computational contributions, not only in the "computational" sessions, but in all relevant fields. Computation is fast becoming an essential instrument in geophysical research.

* A significant number of papers on the high-spin to low-spin transition in Fe which is highly relevant for the properties of the lower mantle.

* Quite a lot of interest in the elastic and plastic properties of the post-perovskite phase of $MgSiO_3$, in relation to the D'' discontinuity.

* Significant research on seismic models which can reveal, by inversion, the composition of the interior of the earth.

Apart from the presentations within these symposia, I visited with interest the posters documenting the state of the art in the use of computers in geophysics, from data acquisition to the handling of large databases, grid execution, and visualization.