Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Iron-based superconductors: What can we learn from DFT? LILIA BOERI, OLEG DOLGOV, Max-Planck-Institute for Solid State Physics, Stuttgart, Germany, ALEXANDER GOLUBOV, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands, OLE KROGH ANDERSEN, Max-Planck-Institute for Solid State Physics, Stuttgart, Germany — The discovery of superconductivity in iron pnictides has initiated an intense theoretical activity. So far, however, not only the pairing mechanism, but even the basic electronic structure of these materials is not well understood. We use Density Functional Theory to understand the electronic and vibrational properties of LaOFeAs, which can be considered a prototype for iron pnictides. First, we calculate the phonon dispersions and electron-phonon coupling using linear response and show that standard Migdal-Eliashberg theory cannot explain the experimental Tc. Then we derive ab-initio an accurate tight-binding Hamiltonian, using downfolding + N-ization (NMTO), which allows us to elucidate the origin of the complicated band structure of iron pnicticides. As a first application of our model, we study magnetism.

Lilia Boeri
Max-Planck-Institute for Solid State Physics

Date submitted: 26 Nov 2008 Electronic form version 1.4