Report of Scientific Activity:

Lilia Boeri

My main research activity involves the study of electron-phonon properties of novel materials, using several Density Functional Theory (DFT) methods. This topic combines the study and extension of the strong-coupling theory of superconductors (*Migdal-Eliashberg Theory*) with ab-initio calculations.

Migdal-Eliashberg Theory has been developed in the 60's-70's to calculate the properties of electron-phonon superconductors in terms of their microscopical properties (Electronic and phononic structure, electron-phonon coupling)[1]. At that time, the relevant quantities were extracted from the available experimental data (specific heat, tunneling, inelastic neutron scattering), which sometimes resulted in a partial or controversial understanding of the systems under study.

Ab-Initio Calculations of the **phonon** dispersions and, later, **electron-phonon coupling** have become feasible due to the introduction of Density Functional Perturbation Theory in the late $80's$ for simple metals and only recently for more complex systems[2].

The field has raisen a renewed interest after the discovery of the 40 K electron-phonon superconductor magnesium diboride (MgB_2) in 2001, which has initiated an intense theoretical and experimental search for new superconductors.

In this framework my research activity has mainly been devoted to the study of the newly-discovered superconductors from first-principles, and in particular to understanding how the crystal/electronic and vibrational structures of these materials are related to each other.

In my PhD thesis, I have shown that the **anharmonic** effects in the phonons of MgB_2 are a general property of systems with degenerate bands, small Fermi energy and strong electron-phonon interaction[3].
I have also given the **first theoretical explanation** for superconductivity in boron-doped **diamond**, silicon and germanium, discovered in 2004, showing that these materials can be seen as a 3D version of MgB_2[4].

In collaboration with experimentalists in the MPI-FKF, I have been working on **electron-doped graphite** (CaC_6), for which superconductivity was observed in 2005; here we have shown that the main parameter that governs the critical temperature is the interlayer distance, which can be modified either by chemical composition or pressure[5-6]. We have also predicted that pressure can lead to structural instability, which has later been confirmed by experiments.

Furthermore, using the newly-developed NMTO method we have been able to understand the nature of the **interlayer states of graphite** and their interaction with phonons in terms of a simple Tight-Binding model, and predicted that electron (field) doped graphite would be superconducting.[7]

Lately I have mainly been working on **Iron Oxypniticides**, which become superconducting with T_c's as high as 55 K. These compounds, based on a layered structure, present strong similarities with the high-T_c cuprates, such as magnetic ordering in the undoped phase. After showing that the $e-ph$ interaction is intrinsically small, and thus cannot be invoked to explain superconductivity[8], we have turned to study possible magnetically ordered phases. We have shown that different DFT methods yield strongly different values of the stabilization energies and magnetic moments, and that these values depend very strongly on the details of the crystal structure. Furthermore, LDA (and GGA) values of the magnetic moments are one order of magnitude larger than those measured by experiment, indicating that many-body effect beyond the standard mean-field description play an important role in this class of compounds [9]. At the moment, we are deriving a first-principles hamiltonian to describe the basic electronic structure of these systems, to use in combination with many-body techniques; we try to identify in this way trends which correlate microscopical details of the electronic structure with the observed differences in T_c's. Other recent projects involve the study of bonding in elemental boron, with the aim of understanding how layered bulk phases of elemental boron can emerge from low-dimensional structures.

Other past projects have involved the calculations of the superconducting properties of the newly-discovered CaAlSi[10], the development of an alternative real-space approach to lattice dynamics (*enatom*)[11], and the calculation of electron-phonon linewidths to compare with the measurements of the new Triple Axis Spectrometer in Garching[12].

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