**Main research interests.**
The field of my main research interest is the first principles study of electronic, magnetic, and transport properties of atomic-size nanosystems. In particular, I am interested in the interplay between magnetism and electron transport in metallic nanocontacts and nanowires consisting of just a short piece of atomic chain suspended between two macroscopic electrodes. Due to small size and reduced dimensionality, these systems often possess very unusual magnetic and electronic properties very different from corresponding bulk samples. In such small systems, the electrical conductance, even at room temperature, is essentially ballistic, when resistive processes of diffusive and inelastic character are negligible, and is proportional to the quantum-mechanical electron transmission at the Fermi energy, $G = \langle 1/2 \rangle G_0 T(E_F)$, where $G_0 = 2e^2/h$ is the conductance quantum. For many metals, such as Au, Cu, or Ar, the transmission function takes values very close to integer numbers (equal to the number of open conductance channels), so that conductance becomes quantized in units of $G_0$.

**Developing the electron transport code.**
In order to calculate quantum-mechanical transmission through atomic-size nanocontacts we have developed few years ago the first-principles density-functional theory (DFT) approach [9]. It uses the plane waves for expanding the electron wave functions and works with both norm-conserving and ultrasoft pseudopotentials (describing atomic cores). The method is implemented in PWCOND code which is a part of the open source electronic structure package Quantum-ESPRESSO, see http://www.quantum-espresso.org. The code has been recently generalized [7] to deal with non-collinear magnetism and to account for spin-orbit coupling (which is expected to become important in heavy 5d metals, such as Pt, Au, Ir etc.), when the electron states should be described by general two component spinor wave functions.

Our method was first applied to study spin-dependent electron transport in ferromagnetic Ni and Co nanocontacts and nanowires [8-10].

**Emerging magnetism and "colossal" anisotropy in monatomic Pt nanowires.**
During the last year I was mainly concentrated on the study of electronic, magnetic, and transport properties of monatomic Pt nanowires and nanocontacts [3,6]. Our interest to monatomic Pt nanowires was motivated by several reasons. First, it has been shown [R. H. M. Smit et al., PRL 87, 266102 (2001)] that short segments of monatomic Pt chains (up to 5 atoms long) can be formed experimentally by a gentle breaking of a thin Pt wire notched in the middle (mechanically-controllable break-junction technique). Second, it has been predicted theoretically [A. Delin and E. Tosatti, PRB 68, 144434 (2003)] that free monatomic Pt nanowires, in contrast to the bulk metal, should exhibit the magnetism already at equilibrium interatomic spacing. The crucial role here is played by spin-orbit coupling. It brings some bands to the Fermi energy (increasing the density of states) and, therefore, makes it easier to violate the Stoner’s magnetic instability criterion for itinerant magnet.

Our goal was to investigate in more details the origin of magnetism in Pt monatomic wire and to address, in particular, the issue of magnetic anisotropy - dependence of various properties, such as the total energy or the conductance, on the magnetization direction. We found [3] that free monatomic Pt nanowires possess a new unconventional feature, which we called colossal magnetic anisotropy (CMA). It consists of the strict impossibility of magnetization to rotate from the parallel to the orthogonal (to the wire axis) direction. This differs radically from the usual case of giant magnetic anisotropy, where magnetization will exist along any directions, although at a direction-dependent energy cost. The effect of CMA in Pt nanowire shows up in a quite broad range of interatomic distances $2.2 \text{ Å} < d < 2.6 \text{ Å}$, including also the equilibrium interatomic distance $d_0 = 2.35 \text{ Å}$. Only
above $d \sim 2.6 \, \text{Å}$ a perpendicular magnetization will finally set in, and CMA will gradually revert to a more conventional giant magnetic anisotropy. The origin of CMA was analyzed in terms of quantum-mechanical selection rule, where the two-fold degenerate electron band (with $m_j = \pm 5/2$, the total angular momentum around the wire axis), crossing the Fermi level and so mainly responsible for the onset of magnetism, can only exchange split by a parallel magnetization but not by a perpendicular one. The splitting of the $m_j = \pm 5/2$ band leads to the magnetic energy gain proportional to the spin moment, similar to the Jahn-Teller effect.

**Ballistic conductance and anisotropic magnetoresistance in Pt nanowire contacts.**

We also studied [6] magnetic properties and ballistic conductance of short monatomic Pt nanowires (3, 4, 5 atoms long) brought in contact with two semi-infinite (nonmagnetic) Pt leads. Here, we considered strained nanowires with a quite large interatomic distance of 2.65 Å, where CMA is already gone. It has been found that for long wires (4 and 5 atoms) both magnetic states exist even in the presence of nonmagnetic bulk leads while for a short 3-atom wire only the state with parallel magnetization survives. We further looked at the ballistic conductance and, in particular, at the effect of anisotropic magnetoresistance (AMR) which is the change in conductance with the magnetization direction. It is characterized by the ratio $(G_\perp - G_\parallel)/G_\parallel$, where $G_\parallel$ and $G_\perp$ are the conductances for parallel and perpendicular magnetizations, respectively. AMR was found to increase with the number of atoms in the wire (in correspondence with the stronger magnetism) and reaches its maximum value of $\sim 15\%$ for the 5-atom nanowire. This value is, however, smaller than the ideal one, $\sim 28\%$, predicted just from the band structure analysis of an infinite nanowire by counting the number of available conductance channels (the number of bands crossing the Fermi level).

**Magnetic impurity on a nonmagnetic substrate: magnetism and electron transport.**

Our particular interest is currently related to the case of magnetic impurities (e.g., Ni, Co, or Fe atoms) placed on some nonmagnetic conductor (such as gold nanowires, carbon nanotubes, graphene etc.), a typical setup for the Kondo problem. We combine the DFT and NRG (Numerical Renormalization Group) approaches to tackle this problem [1]. We studied recently [4] monatomic Au nanowires with a Ni atom adsorbed at different positions. Our DFT calculations show, in particular, that the magnetic moment of the Ni atom depends dramatically on the adsorption site: it is $1 \mu_B/2 \mu_B$ for on side / substitutional geometries. Moreover, the sign of the effective exchange coupling between the spins of conduction electrons and of the Ni impurity is antiferro (predicting a regular Kondo effect) in the bridge case, but ferro (predicting local moment formation) in the substitutional one. These Kondo phenomena can be investigated by building appropriate Anderson models which reproduce the DFT phase shifts and which we solve via NRG [1]. Our NRG calculations predict the zero-bias conductance anomalies very different for the two adsorption cases.

**Some prospectives for the future work**

– A system possessing CMA, unlike most anisotropic nanomagnets, cannot be described even approximately by a spin hamiltonian and is expected to exhibit some novel properties, including a drastic suppression of ordinary spin fluctuations, and of quantum tunneling of magnetization. I plan to work further on the effect of CMA in Pt nanowires and nanocontacts in order to understand better the spin moment dynamics in such kind of systems and its influence on ballistic transport.

– We are also constantly looking for new interesting systems to study. Recently, for example, in collaboration with J. Velev we studied multiferroic tunnel junctions [2] where several layers of ferroelectric material (BaTiO3) were sandwiched between two ferromagnetic bulks (SrRuO3). We found the existence of four states with different directions of magnetization (in the leads) and polarization
having quite different conductances which can be of interest for the future applications. We are currently exploring the influence of various impurities (atomic and molecular, nonmagnetic as well as magnetic), adsorbed on monatomic nanowires on their magnetic and transport properties [4,5]. Another kind of systems interesting to look at are the magnetic impurities and nanowires deposited on some metallic substrates, where some intriguing electron transport measurements were recently reported (see, e.g., N. Neel et al., PRL 102, 086805 (2009)).

– I also continue developing, improving, and maintaining the PWCOND code. In particular, I would like to work on the inclusion of many particle effects (on the DFT+U level) into our current mean-field DFT scheme. We would like also to add to the current implementation of the code the possibility to treat the nanocontacts at finite voltages for calculating their IV characteristics.

PUBLICATIONS


10. A. Smogunov, A. Dal Corso, E. Tosatti

11. F. Picaud, A. Smogunov, A. Dal Corso, and E. Tosatti

12. A. Smogunov, A. Dal Corso and E. Tosatti

13. A. Smogunov, A. Dal Corso and E. Tosatti

14. Smogunov A.N., Kurkina L.I., Farberovich O.V.

15. Smogunov A.N., Kurkina L.I., Farberovich O.V.

16. Smogunov A.N., Kurkina L.I., Kurganskii S.I.

17. Smogunov A.N., Kurkina L.I., Kurganskii S.I.