INPAC: Focused Scientific Highlights

WP1: Nanosuperconductors

Confined flux matter in different geometries has been investigated in superconducting micro- and nanostructures. Transitions between different vortex patterns have been studied by magnetization, transport and direct local visualization (SHPM) techniques. The superconducting phase boundaries Tc(H) for different geometries were determined experimentally and compared with the theoretical predictions made in the framework of the Ginzburg-Landau (GL) theory.

Magnification effects on the compact vortex-antivortex molecules in a superconducting square with magnetic dot were predicted on the basis of the GL equations. These effects are useful for a direct detection of the symmetry-induced antivortices in symmetric superconducting nanostructures. Two-component order parameter superconducting discs were investigated in the framework of the GL theory. Novel vortex phases with different vorticities for the two sub-components of the order parameter have been found.

Superconducting Ga nano-inclusions, created by annealing doped GaAs, were obtained and found to form a percolating network of nanoislands coupled via the Josephson effect. Ion implantation was successfully used to obtain superconducting Pb nano-inclusions.

Periodic arrays of asymmetric nanoengineered pinning centers (antidots) were systematically used to study the vortex ratchet effects. We have found multiple sign reversals of the ratchet effect which have been shown to be caused by the interactions between the vortices attempting to occupy the same pinning site.

WP2: Nanomagnetism

Training and asymmetry in CoO/Co exchange bias systems are shown to result from misalignment between the ferromagnetic Co magnetization and the uncompensated magnetization of the granular CoO antiferromagnet.

By mapping of the local density of states (low-T STM/STS) on nanosize Co islands on Au(111) films, electron standing wave patterns have been resolved on top of the atomically flat islands. The patterns fit to the calculated wave functions for a single electron in a box.

Enhanced Landau-Zener tunneling induced by pulsed fields in Molecular Magnets (Mn12, Fe8) has been observed.

A double hysteresis loop behavior was observed in films consisting of ferromagnetic Co clusters embedded in a thin antiferromagnetic CoO matrix. Such magnetization behavior is related to the presence of two ferromagnetic parts with antiparallel orientations of their magnetization vectors, and is explained in terms of both the exchange bias and exchange spring effects.

The Fe-Fe interlayer coupling across an FeSi spacer layer was directly probed with nuclear resonant scattering of synchrotron radiation. It is shown that static magnetic ordering in the spacer leads to suppression of the coupling at low temperatures. Above 150 K, fluctuating moments in the spacer result in biquadratic coupling.

Upon ion irradiation of epitaxial Fe-films, the surface develops a ripple structure which has a profound effect on the in-plane magnetic anisotropy, providing a way to manipulate the easy and hard axes of the film. The resulting anisotropy has been successfully modeled.

We applied new developments in first principles methodology to the prototype problem of hyperfine fields at isolated impurities in Fe: the LDA+U method for strongly correlated lanthanides in Fe, and hybrid exchange-correlation functionals for actinides in Fe.

WP3: S/F Hybrid nanosystems

Tunable field-induced superconductivity has been observed in superconducting films with a periodic array of magnetic dots with magnetization which is varied by using different hysteresis cycles to magnetize the dots. As a result, the shift of the Tc(H) curve to higher fields of a certain polarity ("magnetic bias") can be controlled by tuning the strength of the field emanating from the dots and compensating the applied field.

Static vortex patterns and dynamic effects, such as guided vortex motion and vortex ratchet effects, were studied in the superconductor/ferromagnet hybrids consisting from the superconducting film covered by magnetic dots, bars, loops with the in-plane magnetization. In-plane magnetic dipoles create asymmetric pinning sites responsible for the appearance of the magnetic dipole vortex ratchets theoretically predicted by Carneiro and now found experimentally. Switchable flux pinning landscape has been created by tuning the magnetic states of the in-plane magnetized loops.

Magnetic domains in ferromagnetic films and bulk substrates were successfully used as magnetic templates highly suitable for the manipulation of the superconducting condensate in the S/F hybrids. Different novel superconducting states were found and investigated in details: domain wall superconductivity and reverse domain suoperconductivity, which were both directly visualized by using local LT scanning laser microscopy.

WP4: Carbon nanosystems (first version)

In view of the ongoing experimental studies of confinement in 2D structures, a general analytical tool was developed to describe the eigenstates in a quantum box of arbitrary shape. The method uses the particle on a disk solutions, which are deformed to cover the shape of the box. A deformation functional was developed which provides convergence and smoothness of the solutions. The method was successfully applied to the spectra of Co-islands in the form of a truncated triangle on a gold surface. In the near future extensions are planned to deal with superconducting pentagons and hexagons.

Using quantum chemical calculations, we have shown the strong influence of doped-metal atoms on geometrical and electronic structures of the silicon, germanium, copper and silver clusters. In some special cases, the doped clusters are stabilized due to the σ-aromaticity or three-dimensional aromaticity.

Carbon nanotubes and nanowalls were studied by scanning probe techniques.

WP5: Silicon nanosystems (first version)

For the first time a comparison has been made between atomically abrupt interfaces of Si single-crystals with nm-thin layers of transition metal (Sc_2O_3) or rare-earth (Lu_2O_3, Gd_2O_3) insulating oxides in amorphous and crystalline (bixbyite) phases. The oxide crystallization is found to result only in a variation of the oxygen-derived valence band energy while the conduction bands derived from the unoccupied d-states of metal cations remain at the same energy.

The effect of crystallization on the band structure is observed in the non-oxide insulator (AlN) deposited on Si upon transition from the amorphous to the hexagonal phase, using IPE, PC, and SE spectroscopy. The conduction band energy is found to be the same as in deposited amorphous alumina, indicating the states derived from s and p states of Al cations are insensitive to the kind of cation involved.

Demonstration by ESR of the absence of an SiO_2-type interlayer in the (100)Si/a-$LaAlO_3$ entity. As this is maintained up to ~850 °C, revealing a thermally most stable and abrupt interface, the $LaAlO_3$ high-κ insulator would thus on these grounds qualify as a suitable insulator for future technological applications.

Mapping of paramagnetic point defects in phase separated SiO/SiO_2 superstructures composed of regular arrays of crystalline Si nanoparticles (~2 nm across) embedded in an a-SiO_2 matrix reveals the presence of a dominant P_b-type interface trap system. Identification of the latter as a purely P_{b0}/P_{b1} system suggests the nanocrystalline particles to be principally bordered by (100)-type facets. Controlled suppression of these centers has enabled to incontestably demonstrate the QC origin of photoluminescence, which can reversibly switched between QC or defect originated.
The intrinsic point defect density in Si/SiO_2 entities thermally grown on biaxially tensile strained Si is found to be distinctly reduced as compared to standard entities, providing a fundamental explanation for the observed enhancement in the strained-Si channel mobility as well reduction in 1/f noise.

Detection of a first dopant (donor) impurity in a high-κ insulator (HfO_2) currently being introduced in the 45-nm technology node. On the basis of revealed hf structure, it has been identified as P_2-type defect, a P substituting a Hf atom in the monoclinic HfO_2 phase, which center will inherently operate as a detrimental charge trap.

WP6: Materials for nanophotonics

WP6a: adding magnetic contribution to the optical response:
A precise way of determining Faraday rotation from both thin molecular films and nanoparticles in a molecular polymer matrix has been developed and allows for the

Faraday rotation spectra in the visible range. In addition, MSHG contrast from superparamagnetic nanoparticles was measured.

WP6b: nonlinear optics of DRONPA Green Fluorescent Protein:
We have finished the experimental study of the second-order nonlinear optical properties of the DRONPA protein, a protein very similar to Green Fluorescent Protein (GFP). Theory confirms the unexpected experimental findings. Dronpa and its mutants have also been used for superresolution imaging.

WP6c: photonic crystal heterostructures:
We have succeeded in using photonic bandgap engineering for fluorescence suppression in both the temporal and spectral domain, for spectral narrowing of fluorescence and for enhancing the energy transfer in light harvesting systems. We have recently found strong influence of a weak external magnetic field (90 Gauss) on the fluorescence dynamics of magnetic quantum dots (and not for closed-shell organic chromophores) in colloidal photonic crystals.

WP7: M and SM self-assemblies

Nanoporous surface confined networks have been realized. Pore sizes currently range from 2.9 to 5.4 nm. These patterns are guest selective. For a given set of molecular building blocks, specific surface patterns can be created on demand only depending on the concentration of the molecular building blocks. The nature of the surface, being porous or not, can be directed by the presence of appropriate guest molecules.

The self-assembly of a set of molecules under potential control has been probed by electrochemical STM demonstrating that the ordering of water-insoluble amphiphiles can be tuned by the potential at the interface between an aqueous electrolyte and a metallic substrate. Conductive 1D nanosystems have been created by the self-assembly of carefully designed tetrathiofulvalene derivatives at the liquid-solid interface.

Conjugated polymers can show very efficient Faraday rotation. Supramolecular organisation was found to have a significant impact on the Faraday response. Thin films of regioregular poly(3-alkylthiophene)s in which strong supramolecular organisation is present, have Verdet constants on the order of 40000 °/Tm. On the other hand regio-irregular poly(3-alkylthiophene)s with no significant supramolecuar organisation do not show any measurable Faraday response in thin films. Furthermore, the processing conditions of the polymers also play a crucial role. While spincoated films typically show high Verdet constants, melt-processed films have Verdet values that are at least an order of magnitude lower. Also in this case, we believe that a difference in supramolecular organisation could be the main reason for this behaviour.

A new molecular mechanism behind active site communication and substrate activation in a thiamine diphosphate enzyme, i.e. phenylpyruvate decarboxylase, has been proposed (publication in J. Biol. Chem.: see report).Lipoteichoic acid, a natural macroamphiphilic molecule consisting of a non polar lipid anchor and a polar D-analynated poly-glycerophosphate chain, self organizes in micelles. These assemblies are being studied as nanoreactors for chiral synthesis (ongoing Ph.D thesis)