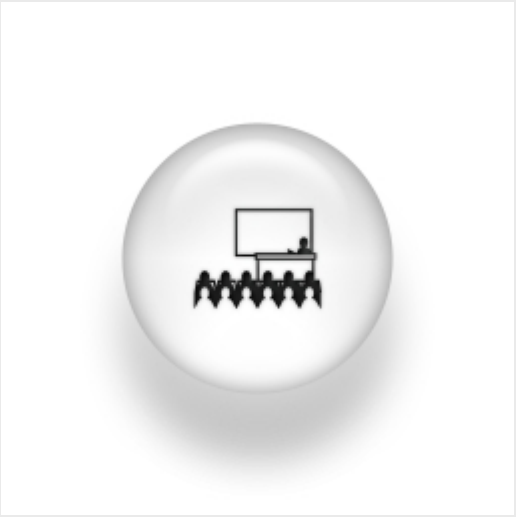
## Theoretical aspects and modelization of low dimensional Molecular Conductors

Monday, 1 October 2007, 12:00-13.00



*Dr. Hitoshi Seo*
Synchrotron Radiation Researh, Hyago, Japan

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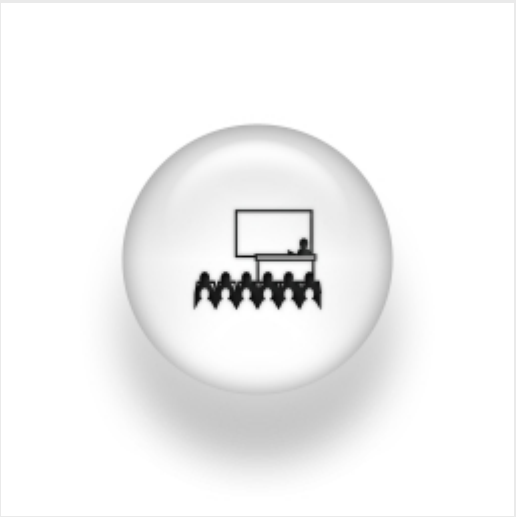
## Adiabatic pumping through quantum dots

Monday, 17 September 2007, 12:00-13.00



*Janine Splettstoesser*
Departement de Physique Theorique, Universite de Geneve
A finite charge can be pumped through a mesoscopic system in the absence of an applied bias voltage by changing periodically in time some parameters of the system. If these parameters change slowly with respect to all internal time scales of the system, pumping is adiabatic.

The scope of this work is to investigate adiabatic pumping through a quantum dot, in particular the influence of Coulomb interaction between electrons in the dot on the pumped charge.
On one hand we develop a formalism based on Green's functions, in order to calculate the pumped charge from the weak-tunnel-coupling regime down to the Kondo regime. We extend our calculations to a system with a superconducting contact.
On the other hand we use a systematic perturbation expansion for the calculation of the pumped charge, giving us the possibility to analyze processes which contribute to charge pumping and to highlight the important role of interaction-induced level renormalization.

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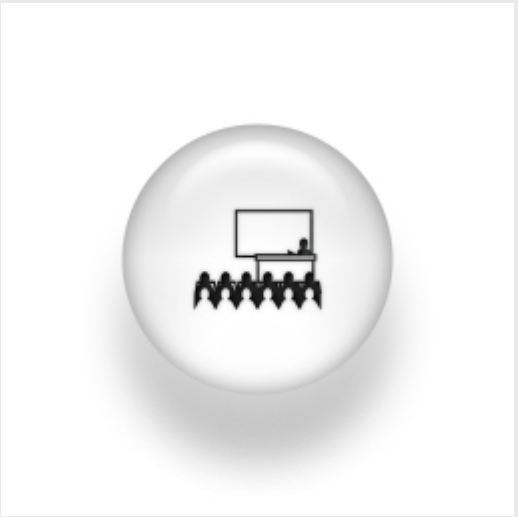
## Hard Superconductivity in Soft Quantum Films

Thursday, 14 June 2007, 12.00-13.00



*Hanno H. Weitering*
The University of Tennessee and Oak Ridge National Laboratory
Superconductivity is inevitably suppressed in reduced dimensionality. Questions of how thin superconducting wires or films can be before they lose their superconducting properties have important technological ramifications and go to the heart of understanding coherence and robustness of the superconducting state in quantum-confined geometries. In this talk, I will show how quantum confinement of itinerant electrons in a soft metal, Pb, can be exploited to stabilize superconductors with lateral dimensions of the order of a few millimeters and vertical dimensions of only a few atomic layers. These extremely thin superconductors show no indication of defect- or fluctuation-driven suppression of superconductivity and sustain enormous supercurrents of up to 10% of the theoretical depairing current density. Their magnetic hardness implies a superconducting critical state with strong vortex pinning that is attributed to quantum trapping of vortices. Our study paints a conceptually appealing, elegant picture of a model nanoscale superconductor with calculable critical state

properties and surprisingly strong phase coherence. Finally, I will show how the quantum growth and superconductive properties of the films can be tailored by Fermi surface engineering, and I will discuss the possibility of multi-gap superconductivity in quantum-confined thin films. This work was done in collaboration with M.M. Ozer, J.R. Thompson, Yu Jia, and Z.Y. Zhang [1,2]. [1] M.M. Ozer et al., Nature Phys. 2, 173 (2006) [2] M.M. Ozer et al., Science, June 15 (2007)

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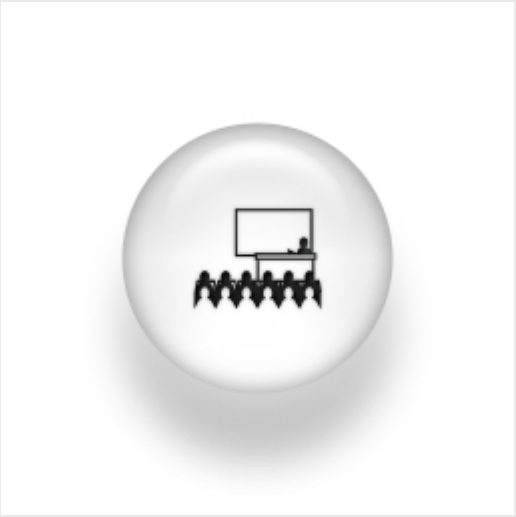
## Adaptive Resolution Molecular Dynamics Scheme

Wednesday, 23 May 2007, 12.00-13.00



*Dr. Matej Praprotnik*
Theory group of the Max Planck Institute for Polymer Research, Mainz, Germany
We have been developing a novel adaptive resolution technique for efficient multiscale molecular dynamics (MD) simulations. The new approach is tailor-made for studying molecular systems that require in some regions an atomistic resolution but otherwise involve length and time scales that are difficult to capture by the conventional atomistic MD simulation. Our method allows an on-the-fly interchange between a given molecule’s atomic and coarse-grained level of description, enabling to reach large length and time scales while spatially retaining atomistic details of the system. The new approach is tested on the model system of a liquid of tetrahedral molecules. The simulation box is divided into two regions: one containing only atomistically resolved tetrahedral molecules, the other containing only one particle coarse-grained molecules. Molecules can freely move between regions while changing their level of resolution accordingly. It is shown that this system has the same statistical properties as the corresponding fully atomistically resolved system at the same physical conditions.