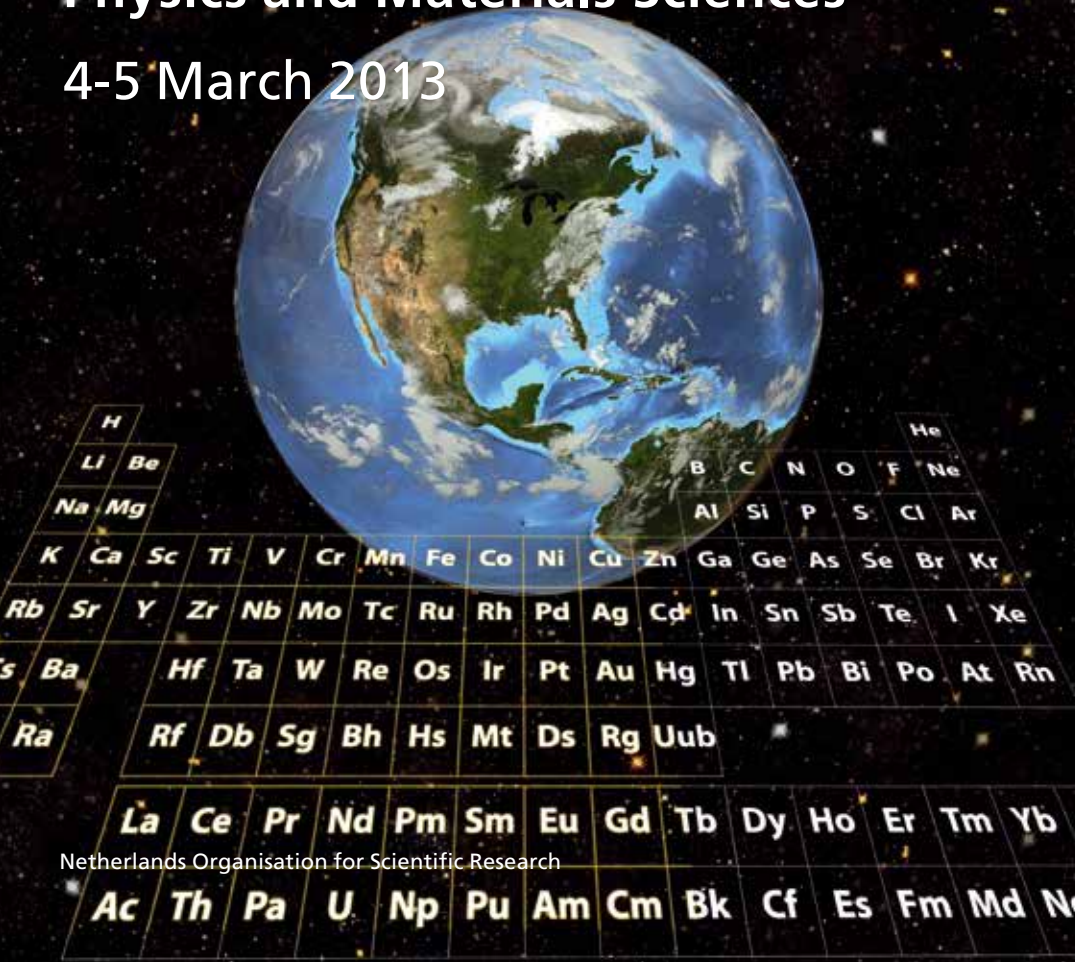
NWO CW Study group meeting

Chemistry in Relation to Physics and Materials Sciences

4-5 March 2013



Netherlands Organisation for Scientific Research

Session 6 – Theory: Physical properties explained by quantum theory

Spin polarized current in Fe(001)|C60|Fe(001) junctions

Author: **Deniz Cakir**
Co-authors: *Diana Otalvaro and Geert Brocks*
University of Twente

Organic spintronics offer the advantage of preserving the spin polarization of carriers, because of the weak spin-orbit interaction in organic materials, hence allowing for robust spin manipulation and readout. In agreement with experimental observations, ab initio calculations reveal an energy dependent spin-polarization at the interface of Fe (001) surface-C60 monolayer, resulting from the hybridization between ferromagnetic Fe d states and C60 n states. By ab-initio calculations we study whether spin polarization at the interface translates into a spin polarized current through a Fe (001)-C60-Fe(001) junction and, by extension, whether this system can perform as a spin filtering device.

Periodic hybrid DFT calculations on the metallic and the insulating phase of (EDO-TTF)2PF6

Author: **Gerrit-Jan Linker**
Co-authors: *Piet Th. van Duijnen, Paul H.M. van Loosdrecht and Ria Broer*
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We present all electron, periodic hybrid DFT calculations on the insulating and the conducting phase of the organic charge transfer salt (EDO-TTF)2PF6. In this material the near planar EDO-TTF donor molecules arrange in stacks. PF6 acceptor molecules reside in cavities between the donor stacks, forming two dimensional slabs. The three dimensional crystal consists of a stacking of such slabs. A one dimensional conduction channel is formed by the overlap of molecular -orbitals of EDO-TTF molecules. We discuss the electronic properties, such as the band structure, the density of states and the Fermi surface, in relation to the metal-insulator transition in this material. The nature of conduction is confirmed in both phases from their band structures and density of states. We discuss the phase transition in terms of a Peierls mechanism, fully in line with our results.