Wigner 121
Scientific Symposium

Wigner Research Centre for Physics
Institute for Solid State Physics and Optics
Department of Theoretical Solid State Physics
Long-range order in condensed matter systems
Research Group

Nóra Kucska, Krisztián Palotás, András Lászlóffy, Levente Rózsa, Balázs Újfalussy

Method

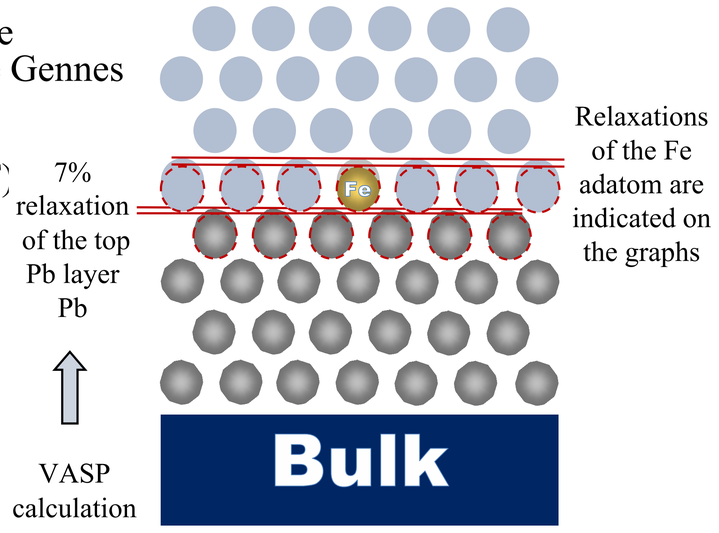
Based on the Korringa-Kohn-Rostoker Green Function (KKR-GF) method by solving

- the Dirac equation for the normal state
- the Kohn-Sham-Dirac Bogoliubov-de Gennes equation for the SC state

within multiple scattering theory (MST)

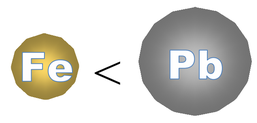
Surface and interface systems
Semi-infinite, inhomogeneous
Semi-infinite Green function can be calculated in MST
(NO supercell)

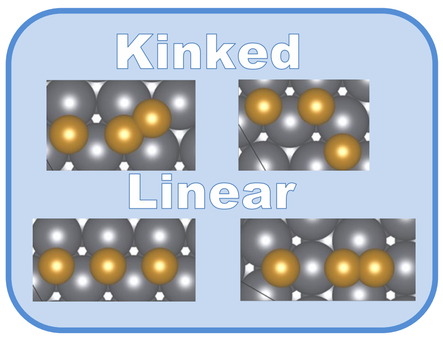
Impurity systems
Bulk, surface impurities, nanostructures



Modelling the experiment

Experimental result for iron clusters:
Spectra of dI/dV for the
(a) single Fe atom,
(b) Fe2 cluster,
(c) linear- and
(d) kinked Fe3 cluster.





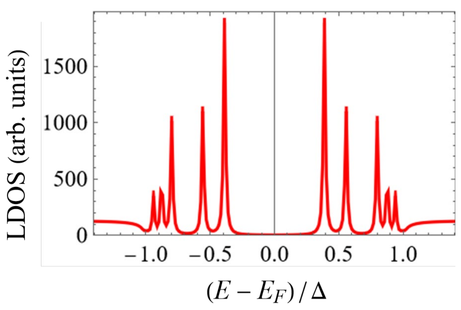
Taking into account
- The surface relaxation
- The position of the impurities (fcc or hcp)
- The shape of the iron cluster
- The tip DOS-, the position of the tip relative to the impurity
- The magnetic moments configuration of the impurities (AFM, FM)

The STM images of the respective clusters acquired with a superconducting Pb tip on Pb(111)
(the DOS-, and the position of the tip relative to the impurity)
Experiment conducted at T= (6.64±0.94)K
by Silas Amann, Nicolas Néel, and Jörg Kröger
Institut für Physik, Technische Universität Ilmenau,
D-98693 Ilmenau, Germany

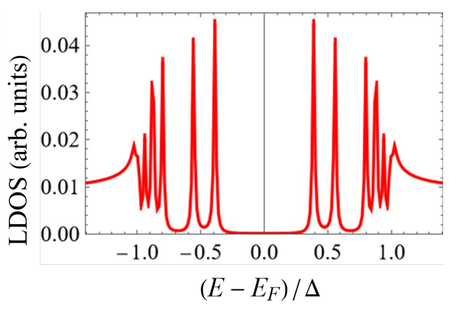
Results

The position of the tip relative to the impurity

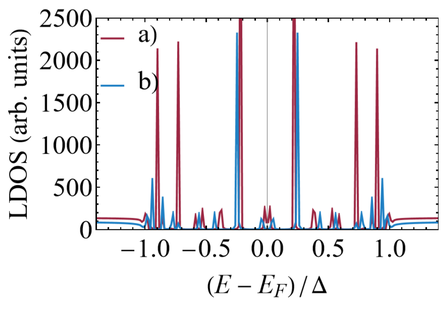
LDOS in the adatom



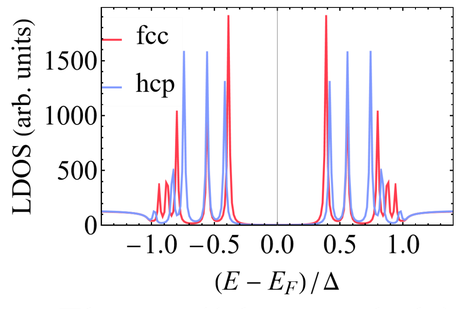
LDOS in the vacuum on top of the adatom



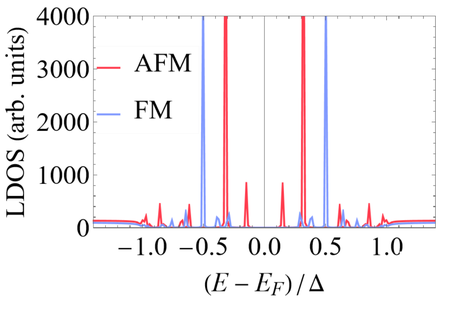
The shape of the iron cluster



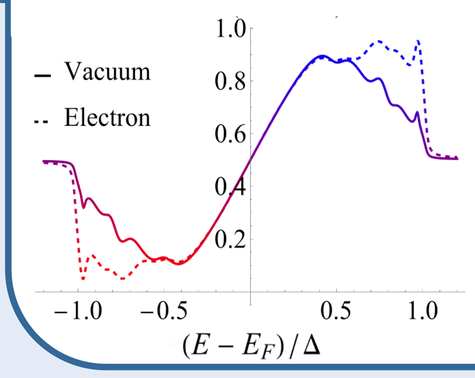
The position of the impurities



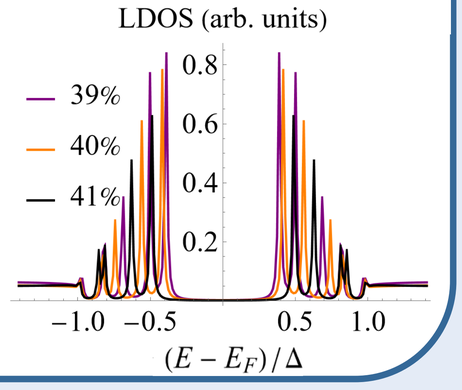
The magnetic moment configuration of the impurities



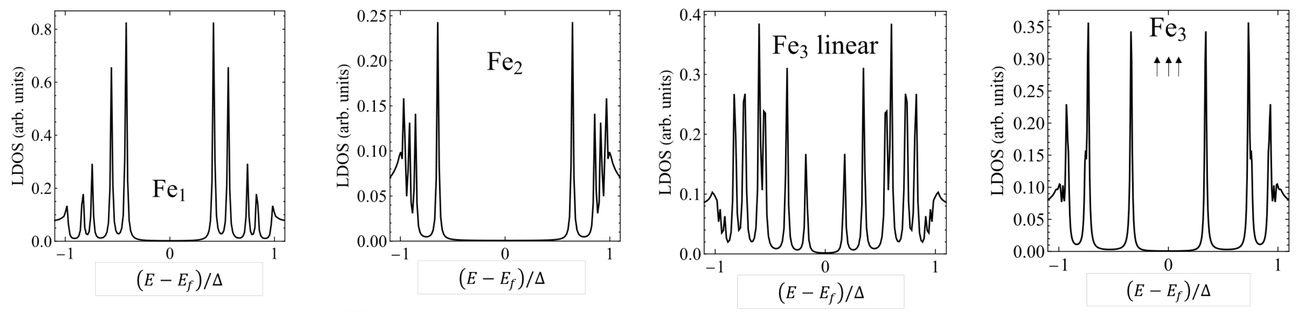
Electron/(electron+hole) ratio



Effects of relaxation



Local density of states



(1) Calculated LDOS is first convolved with ρ_t

(2) Any additional experimental broadening was considered by convoluting dI/dV and a Gaussian function of width σ

(1) Tip density of states

The tunneling current: $I(V) \approx \int_{-\infty}^{\infty} \rho_t(E - eV, T_t)\rho_s(E, T_s)[f(E - eV, T_t) - f(E, T_s)]\mathrm{d}E$

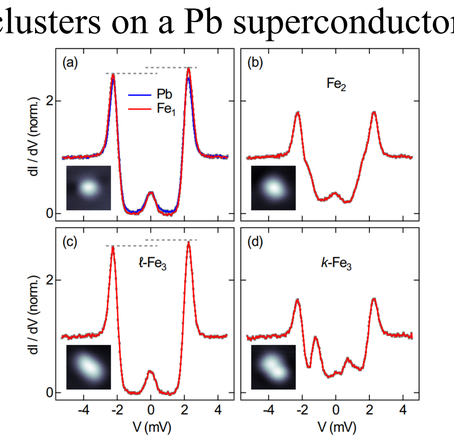
ρ_t and ρ_s represent tip and sample density of states (DOS)

$$\rho(E,T) = \mathrm{sgn}(E)\mathrm{Re}\left[\frac{E + i\Gamma}{\sqrt{(E + i\Gamma)^2 - \Delta(T)^2}}\right]$$

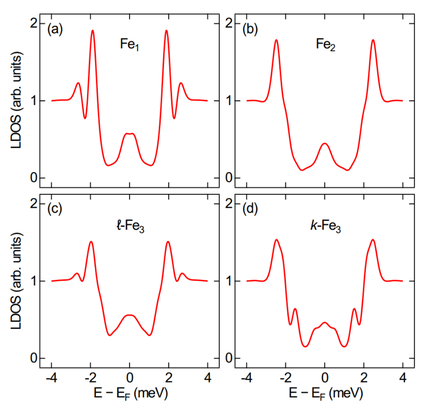
Δ(T): the width of the BCS energy gap
iΓ (i^2= -1): the broadening of the DOS due to the finite lifetime of the quasiparticles
f(E,T): the Fermi-Dirac distribution at given energy E and temperature T
Numerical differentiation yields the differential conductance dI/dV

Experimental agreement

Scanning tunneling spectroscopy of Yu-Shiba-Rusinov states of iron clusters on a Pb superconductor



Convolved LDOS



HUN-REN Hungarian Research Network

MTA Centre of Excellence