Spin-dependent electron excitation and emission in the neutralization of He^+ ions at paramagnetic surfaces

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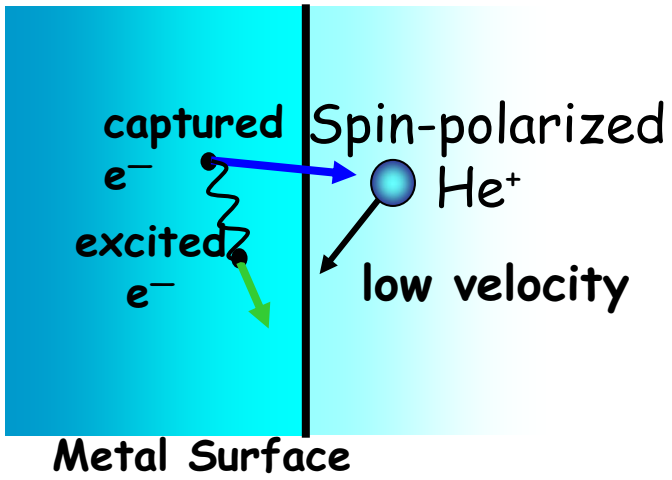
Motivation: Spin polarized He^+ ions on paramagnetic surfaces

Measurements of the spin polarization of the electrons ejected during the Auger neutralization of **spin polarized** He^+ ions impinging on **paramagnetic surfaces**



[1] D. L. Bixler et al., Phys. Rev. B 60, 9082 (1999)
[2] J. C. Lancaster et al. Phys. Rev. B 67, 115413 (2003)

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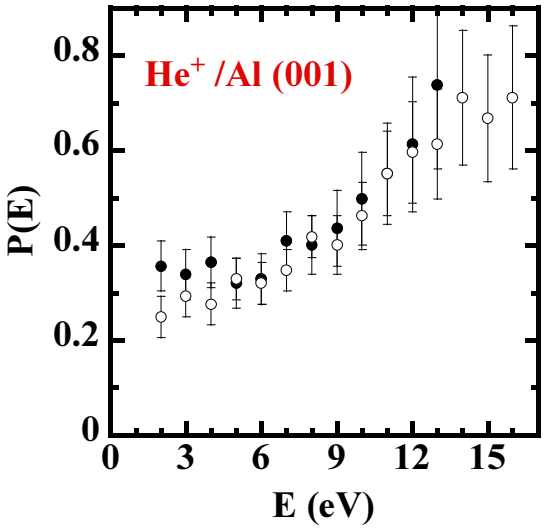
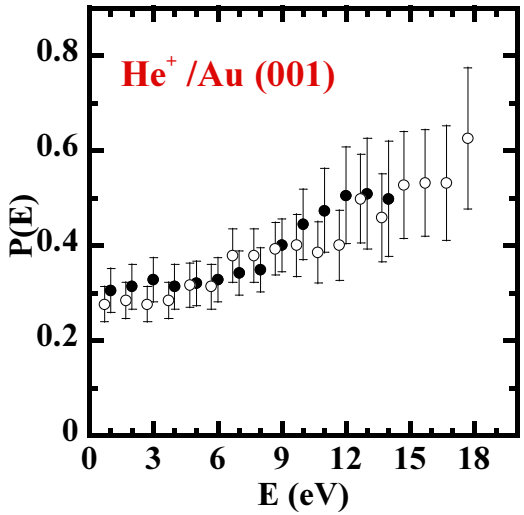
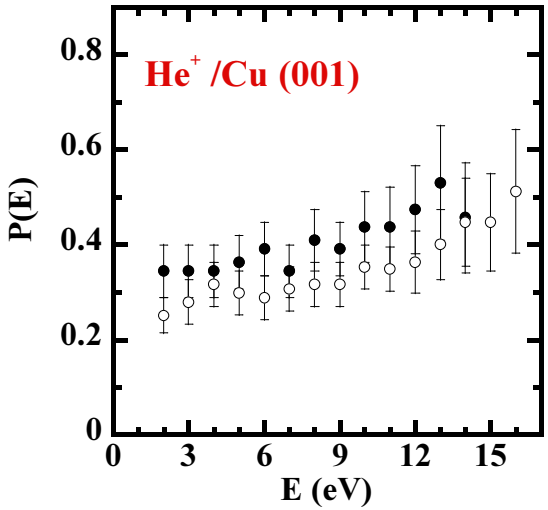






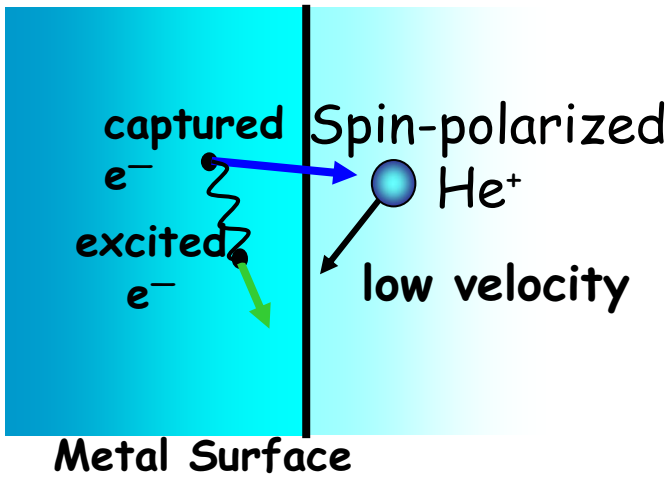
- Similar behaviour of the spin-polarization for

  Al(001) Au(001) and Cu(001)

- Spin-polarization of emitted electrons: ~ 30%

- Spin-polarization larger at higher emission energies: Al > Au and Cu

Theoretical model: 3-step process

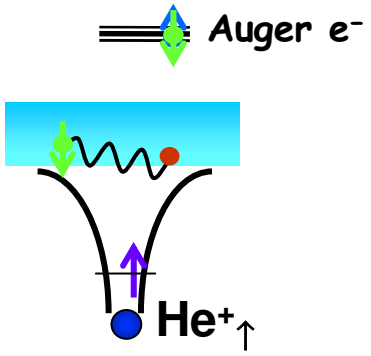


1. Auger neutralization of He+
2. Transport of excited electrons
3. Escape of excited electrons

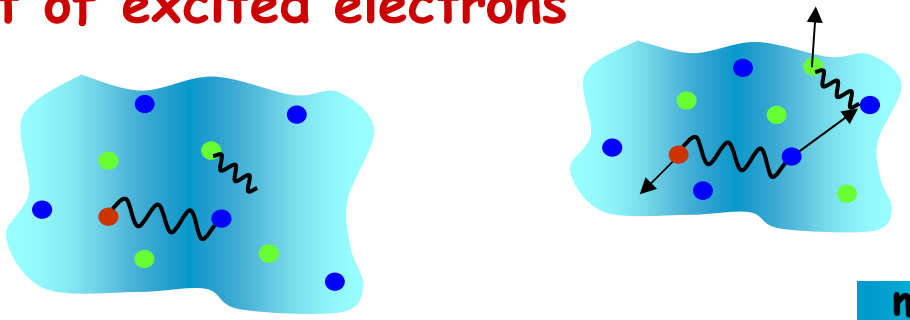
Experimental neutralization distance ~ 2-3 a.u. ⇒ Local model reasonable approximation

Theoretical model: 3-step process

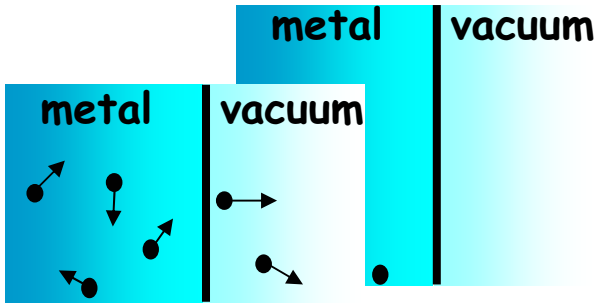
1. Auger neutralization of He+



2. Transport of excited electrons



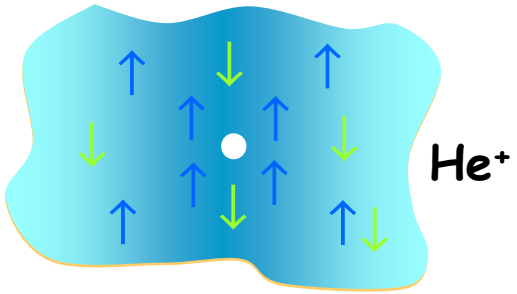
3. Escape of excited electrons



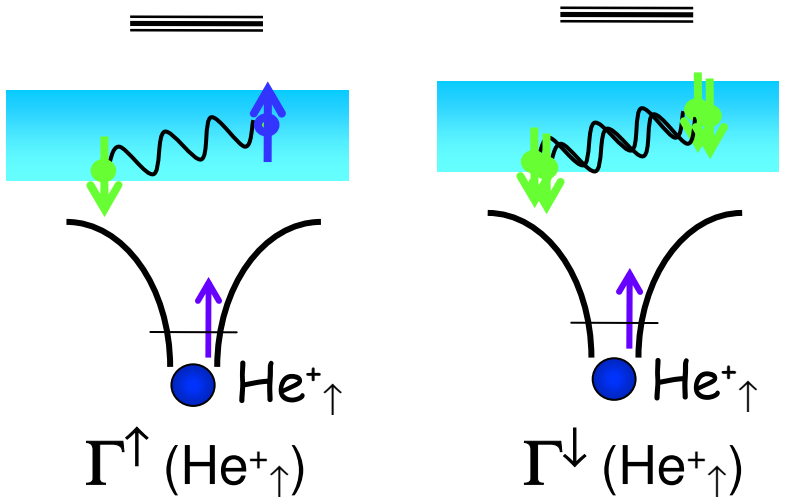
Auger neutralization of He^+:

Ingredients contributing to the spin dependence

Spin-dependent screening of the He^+ ion



Indistinguishability



Theoretical model for the Auger neutralization process

Description of the system: He^+ in FEG

- **Density Functional Theory** and the **Local Spin Density** approximation
- **Kohn-Sham equations** are solved self-consistently for each spin orientation

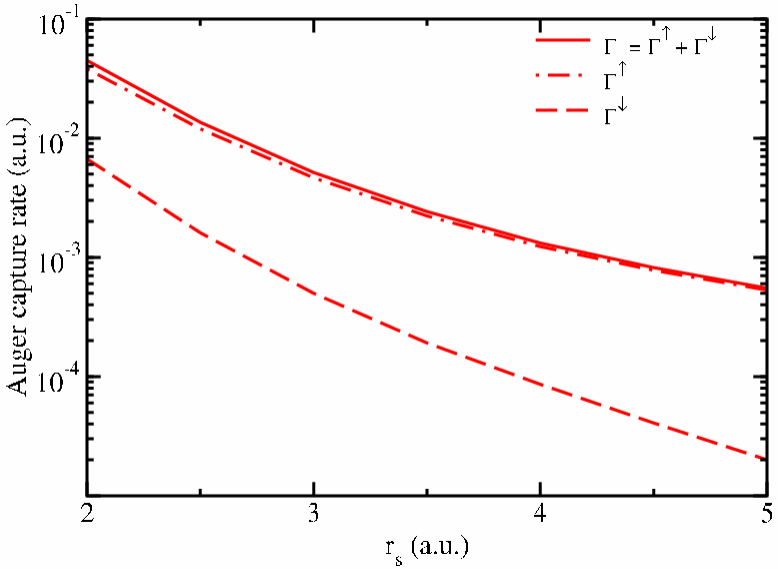
Auger capture rate

- **First-order perturbation theory:** $\Gamma(He^+_{\uparrow}) = \Gamma^{\uparrow}(He^+_{\uparrow}) + \Gamma^{\downarrow}(He^+_{\uparrow})$
- **Initial and final states are described by the Kohn-Sham** $\varphi_i^{\uparrow}(\mathbf{r}), \varphi_i^{\downarrow}(\mathbf{r})$

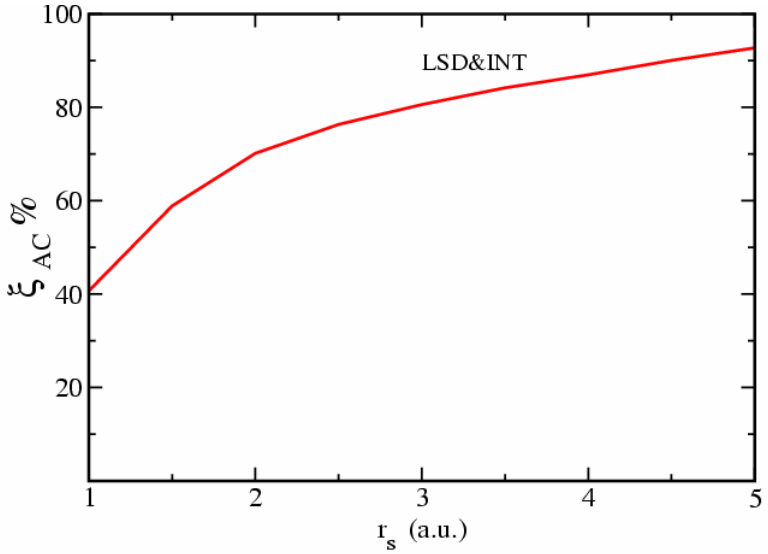
Spin polarization of the AC for He^+ ions

[M. Alducin et al., Phys. Rev. A 70, 012901 (2004)]

AC rates



$$\xi_{AC} = \frac{\Gamma^{\uparrow} - \Gamma^{\downarrow}}{\Gamma^{\uparrow} + \Gamma^{\downarrow}}$$

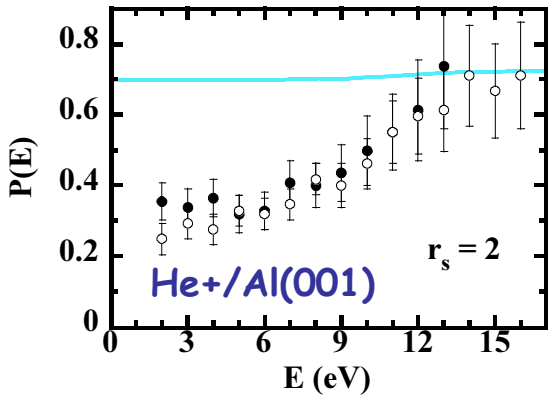


Screening and interference favours the excitation of spin-up electrons

Comparison to experiments: What is missing?

Experimental data	Theoretical results
EMITTED electrons	EXCITED electrons
Spin orientation: parallel to $He^+_\uparrow$	Spin orientation: parallel to $He^+_\uparrow$
Spin-polarization: ~ 30%	Spin-polarization: ~ 60% - 80%

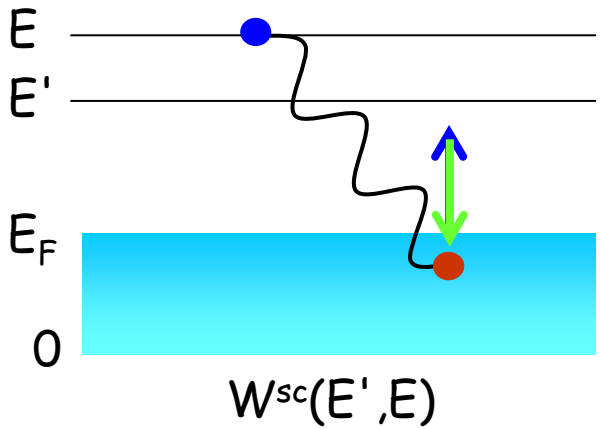
(for typical metal densities)

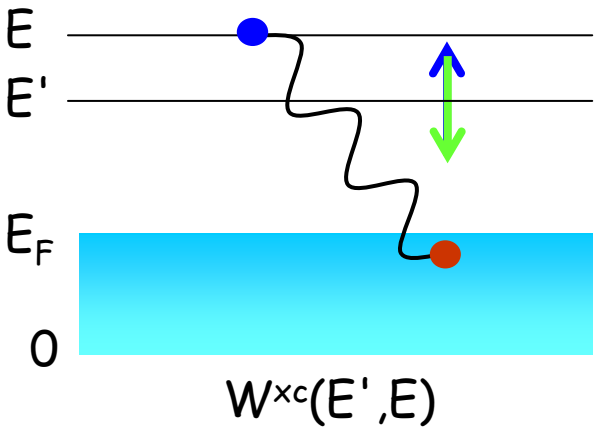


Transport theory of excited electrons

- Boltzmann transport equation in bulk
- Primary electrons: electrons excited during the Auger process
- Secondary electrons created by e^--e^- scattering processes:

Probability: $(E,\sigma) \rightarrow (E',\sigma')$





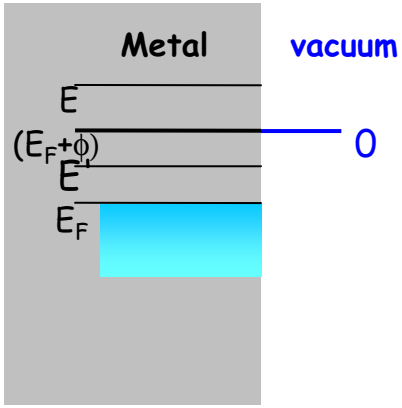
Final distribution of inner excited electrons

Boltzmann transport equation

$$\frac{v(E)}{l(E)} N^{\sigma}(E) = S^{\sigma}(E) + \int_{E}^{E_{max}} dE' \left(W^{sc}(E,E') + \frac{1}{2} W^{xc}(E,E') \right) N^{\sigma}(E')$$

$$+ \frac{1}{2} \int_{E}^{E_{max}} dE' \, W^{xc}(E,E') \, N^{-\sigma}(E'), \quad \sigma = \uparrow, \downarrow$$

Escape of electrons: Step surface barrier



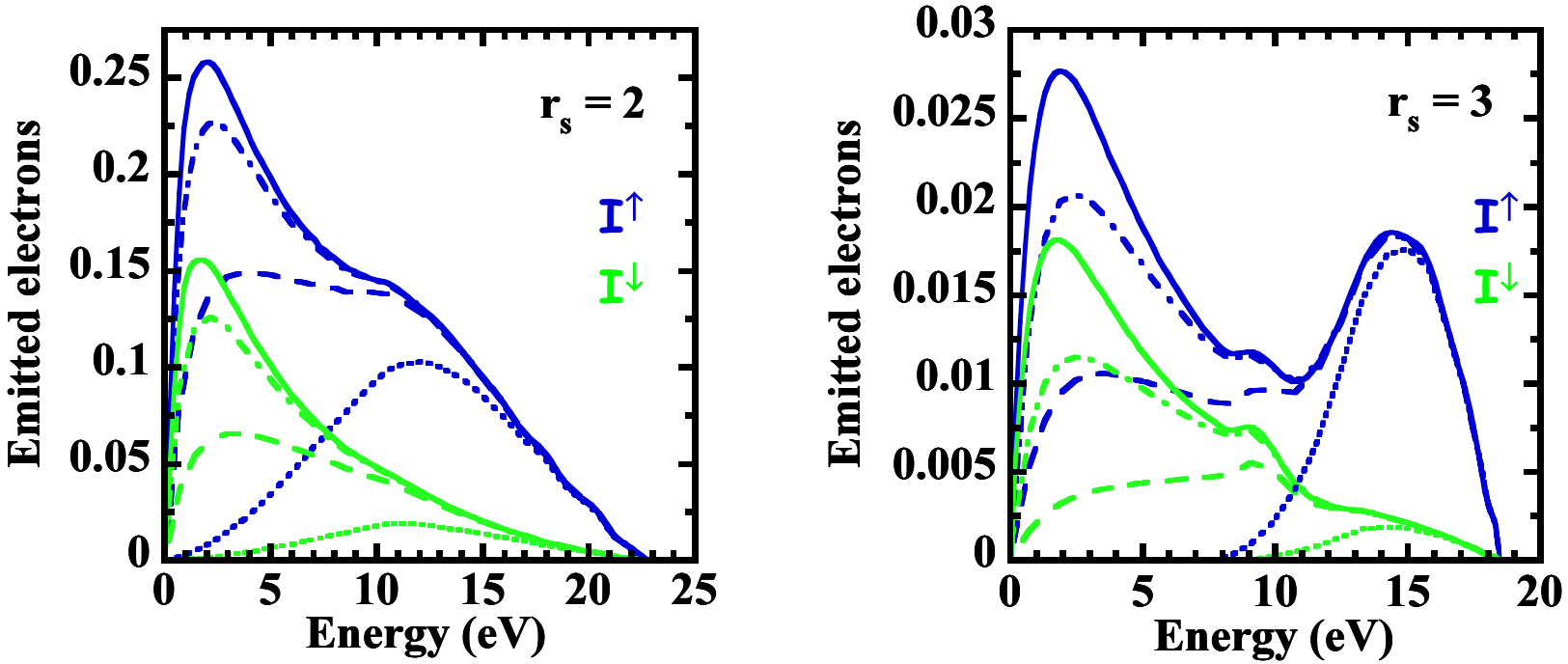
$N^{\sigma}(E) \longrightarrow I^{\sigma}(E)$

distribution of EXCITED e^-

distribution of EMITTED e^-

Energy distribution of emitted e^- $I^{\uparrow}$ and $I^{\downarrow}$

[M. Alducin et al., Phys. Rev. A 72, 024901 (2005)]



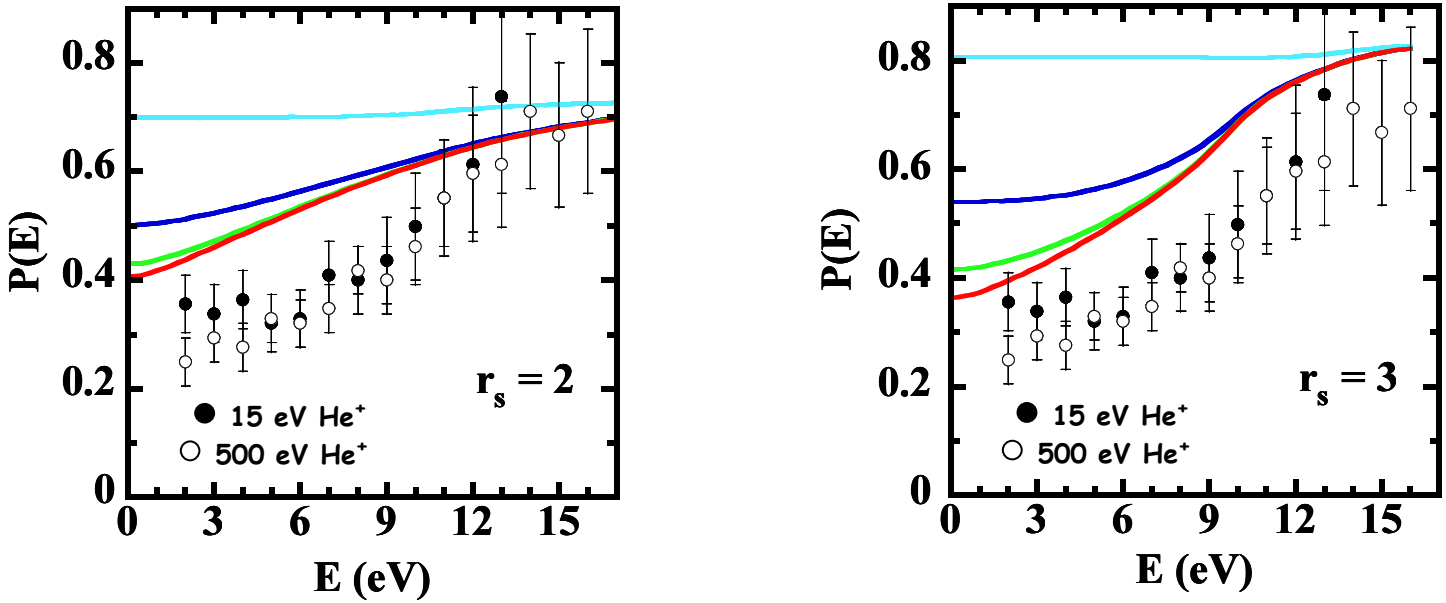
At low E, the number of **emitted** and **excited** electrons differs

At high E, **excited** electrons are ***directly*** **emitted**

Comparison with experiments

Polarization of e^- emitted with energy > E

He^+/Al (001) Al: r_s=2.07



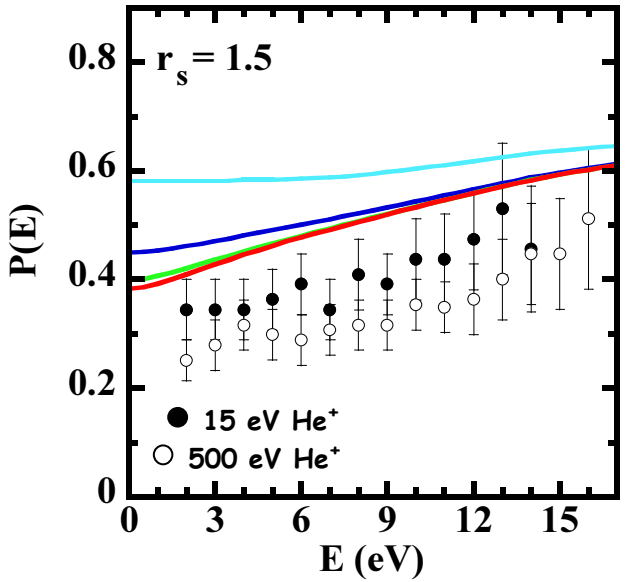
Experimental data: J.C. Lancaster et al. PRB **67**, 115413 (2003)
Theoretical data: M. Alducin et al. PRA **72**, 024901 (2005)

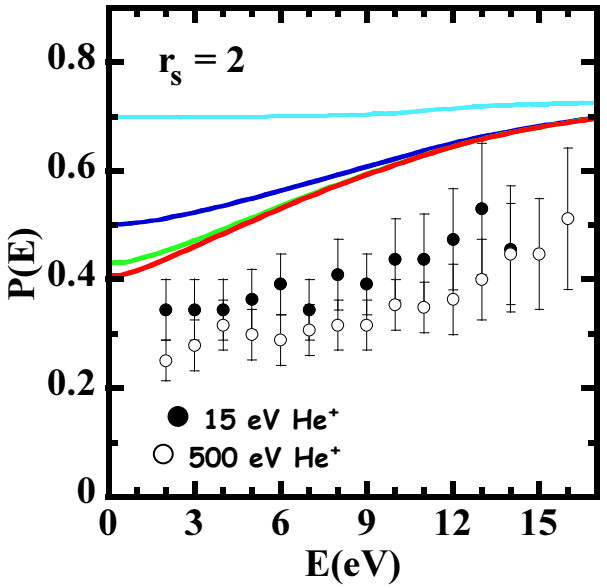
Comparison with experiments

Polarization of e^- emitted with energy > E

He^+/Cu (001)

Cu: r_s=1.83 including *d*-e^-





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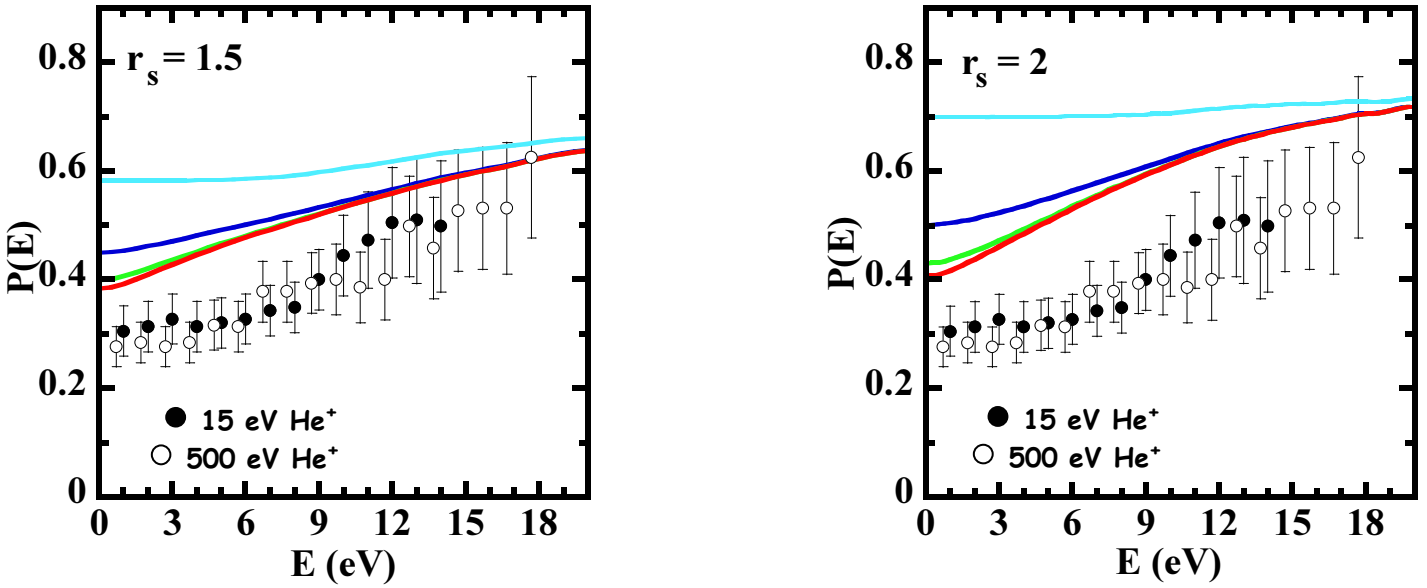
Comparison with experiments

Polarization of e^- emitted with energy > E

He^+/Au (001) Au: r_s=1.49 including *d*-e^-



Experimental data: J.C. Lancaster et al. PRB **67**, 115413 (2003)

Theoretical explanation of the experimental data

Polarization of the total e– yield

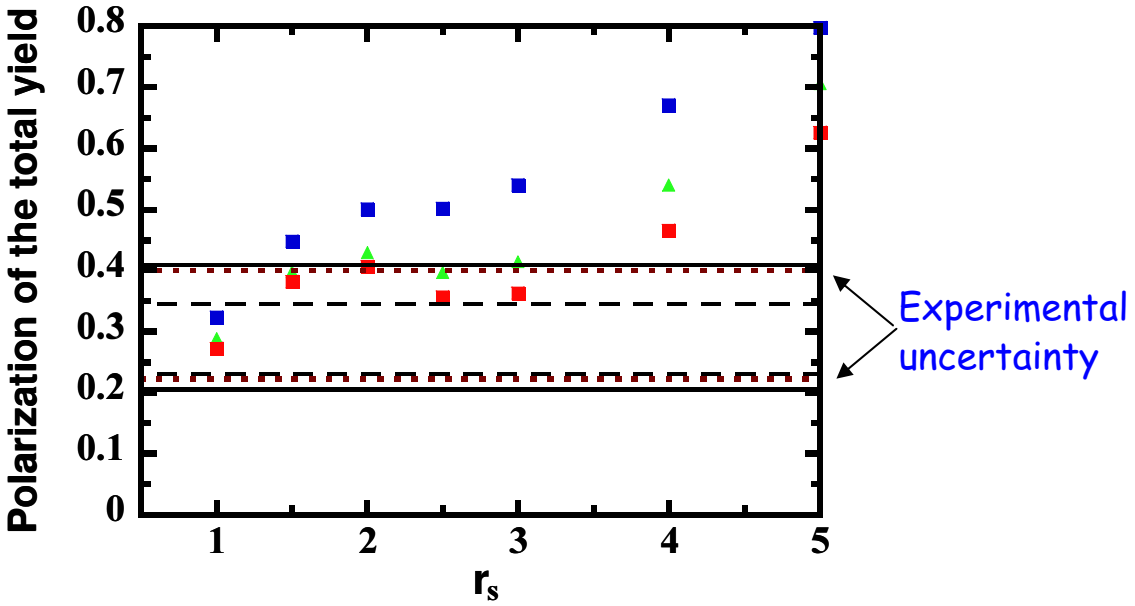
Experiments

Similar value of ~ 0.3±0.1
for Al(001) Au(001) Cu(001)

Theory

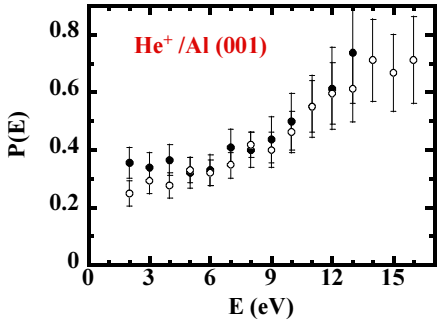
For r_s<4,
P(0) hardly depends on r_s

Slight variations on P(0)
are within the
experimental uncertainty

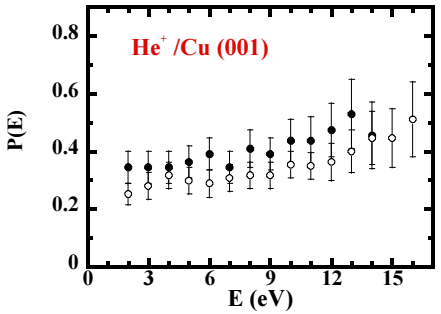


Theoretical explanation of the experimental data

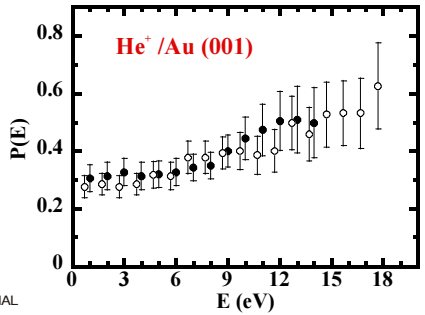
Polarization of e- emitted at high E



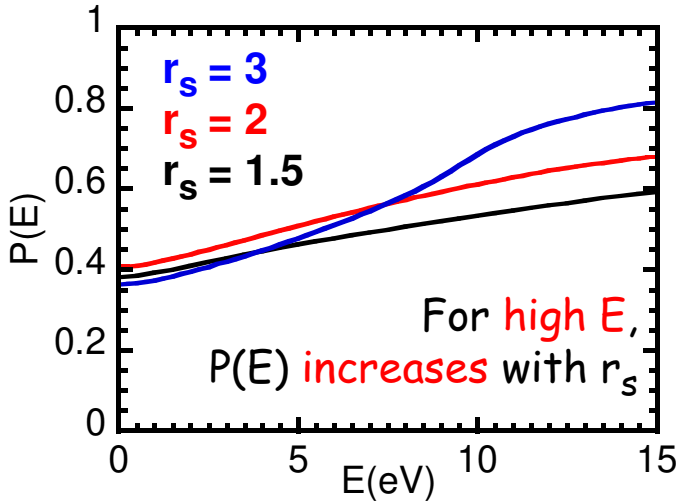
P(E) ~ 70%



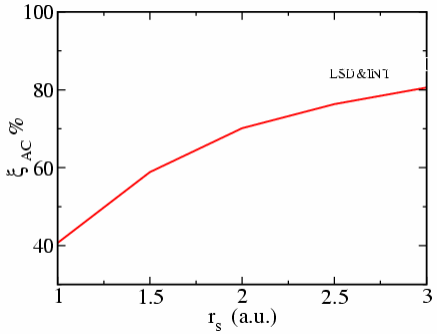
P(E) ~ 50%



P(E) ~ 50%



Spin polarization of AUGER excited electrons



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Summary

Our theoretical model allows us to **explain** the measured **spin polarization of e^- emitted** during the neutralization of He^+ ions on paramagnetic surfaces:

1. The spin orientation of emitted e^- is governed by the highly spin-dependent **Auger neutralization** process

2. The **transport process** is responsible of reducing the high spin polarization of Auger (excited) e^- down to the experimental 30%
   In particular,
   - **At low E,** the spin polarization is strongly reduced
   - **At high E,** the spin-polarization of emitted e^- confirms the strong spin polarization of the Auger e^-
3. Spin polarization of the total yield almost independent of r_s in agreement with the similar values found for Al (001) Au (001) Cu (001)
4. r_s-dependence only observed at high E, P(E) larger for Al(001), the surface with a lower electron density (Al: rs=2.07, Cu: rs=1.83, Au: rs=1.49)