# Electronic Stopping of slow H and He in gold from first principles

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# Outline of this talk

- Electronic stopping power
- Electronic stopping in Jellium
- Electronic stopping in metals: simple vs transition metals
- Our TDDFT calculations on gold using SIESTA

# Electronic Stopping Power

- A charged particle moving through a solid material interacts with it and loses its kinetic energy to both the electrons and the nuclei inside it.
- Amount of energy given to electrons per unit distance is called electronic stopping power.

# Electronic stopping in Jellium

- For a slow moving projectile, the electronic stopping is proportional to the velocity of the projectile.

- The proportionality constant depends on the projectile and the density of electrons in the jellium.

# What do Experiments find?

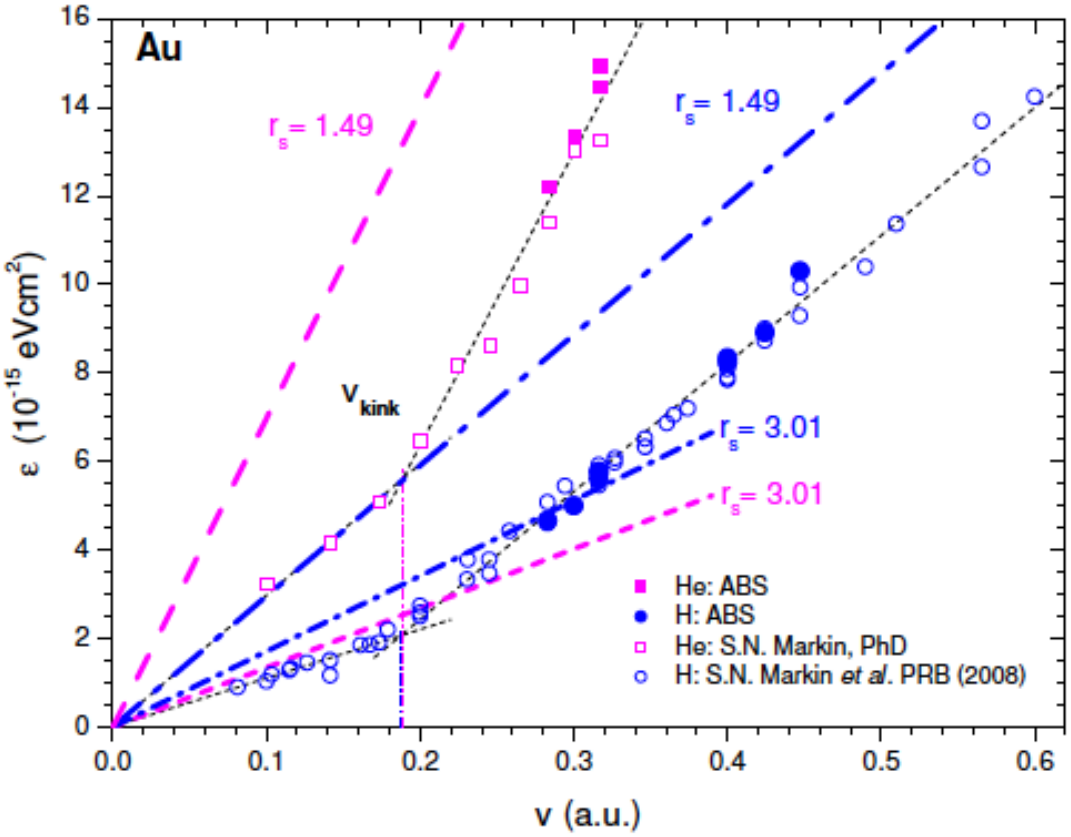
## Do metals act like a jellium?

✓ Sp-bonded metals, e.g., Al : $S \sim v$

✘ Transition metals, e.g., Cu: slope increases around v = 0.1- 0.2 a.u.

# An Example: H and He in gold

PHYSICAL REVIEW B **80**, 205105 (2009)




$\varepsilon = S/n_a$

$r_s \sim 1/n^{1/3}$

.., $5d^{10}$, $6s^1$

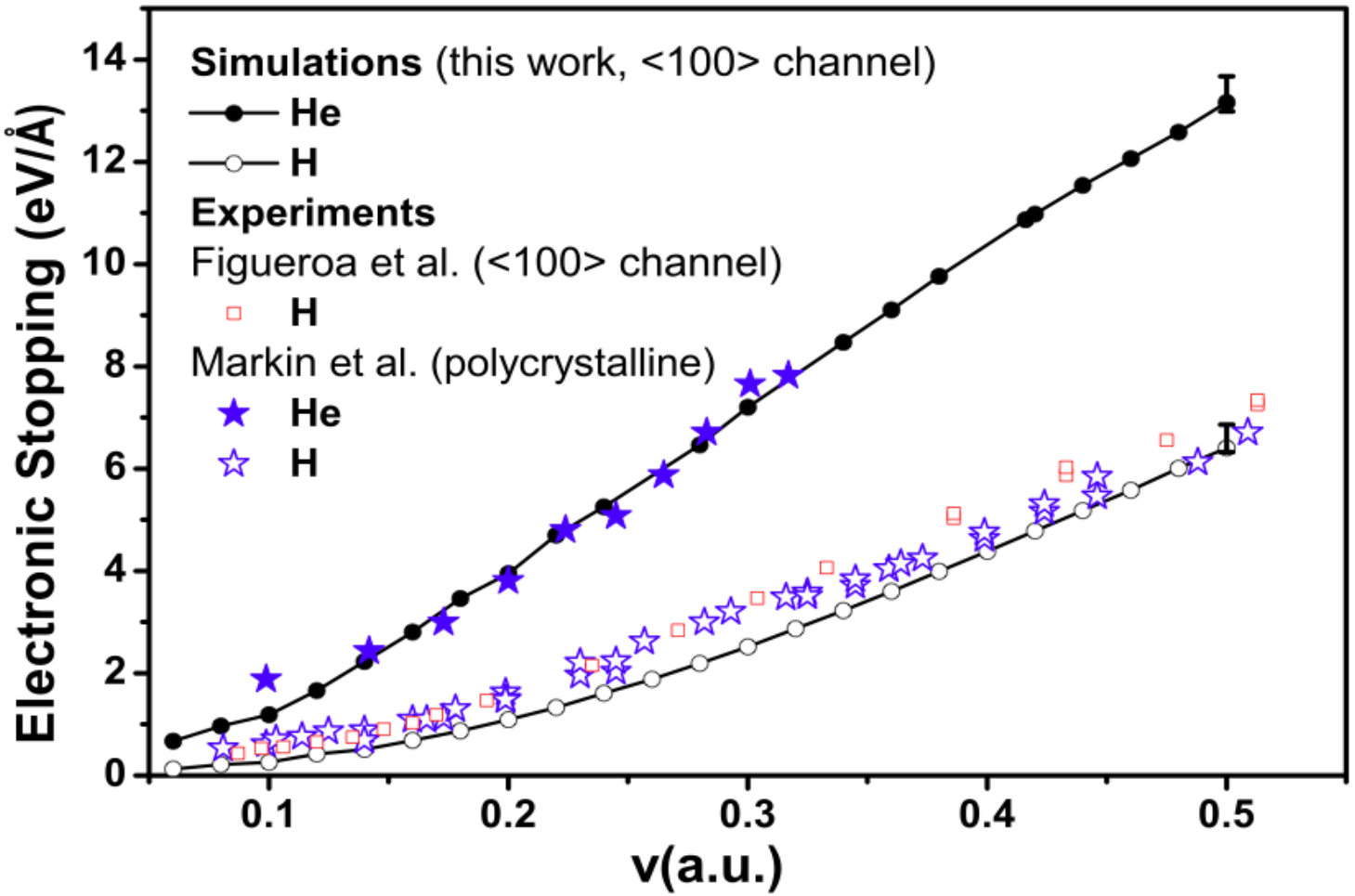
DFT: Echenique et al.
Solid State Communications, 37, 779 (1981)

# Our calculations

- Ehrenfest Dynamics
- Electrons - Quantum Mechanics

  Time Dependent Density Functional Theory
- Ions - Classical Mechanics

# Results


Simulations (this work, <100> channel)
He
H
Experiments
Figueroa et al. (<100> channel)
H
Markin et al. (polycrystalline)
He
H
Electronic Stopping (eV/Å)
v(a.u.)
0
2
4
6
8
10
12
14
0.1
0.2
0.3
0.4
0.5

# Condor Script

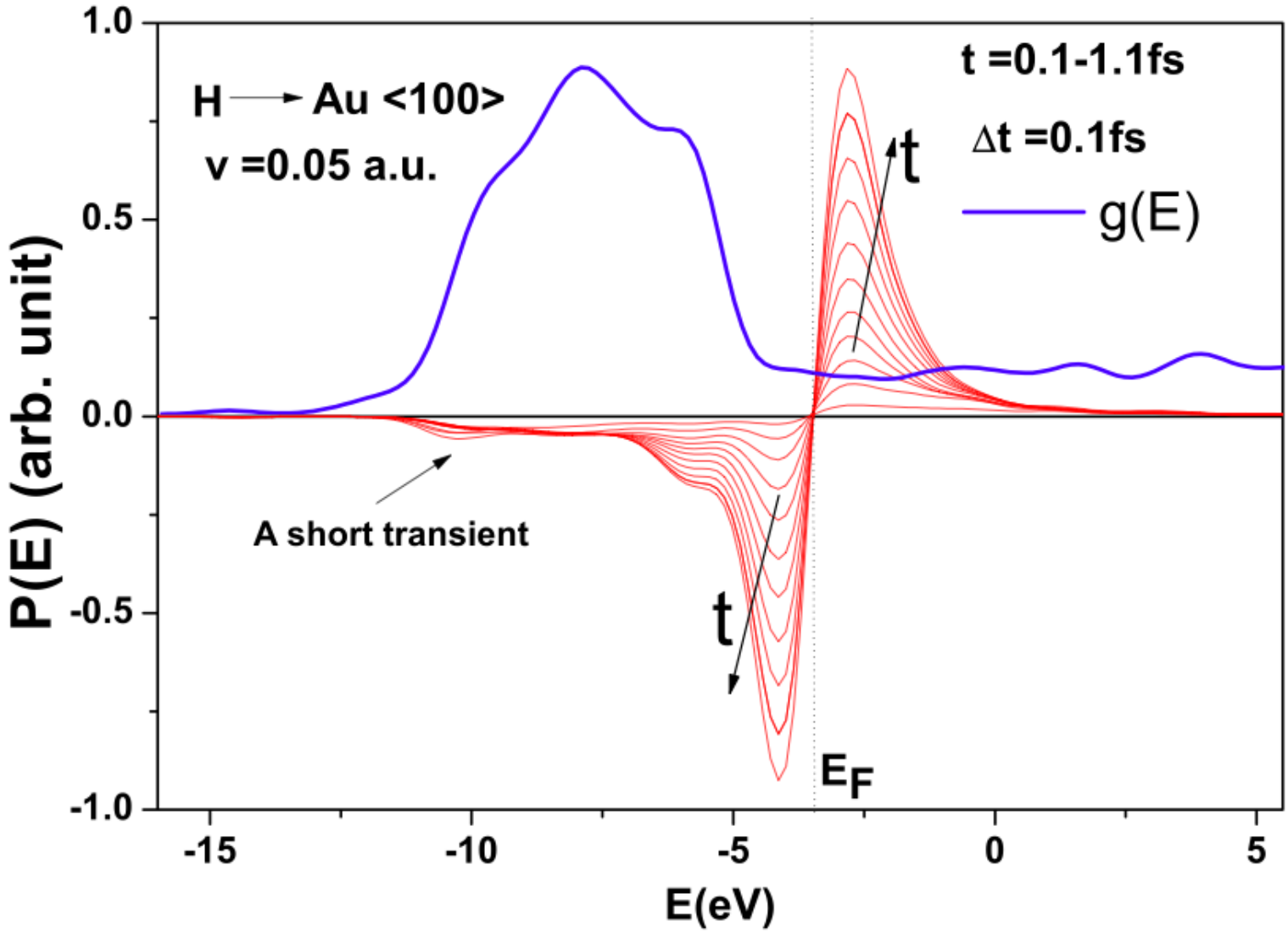
```
Universe = standard
Executable = /home/maz24/siesta-25april11
Input = AuH.fdf
transfer_input_files  =
Au.psf,H.psf,AuH.XVi,AuH.VERLET_RESTARTi,AuH.DM,
AuH.TDWF,AuH.etot_vs_time
should_transfer_files = YES
when_to_transfer_output = ON_EXIT_OR_EVICT
Requirements = OpSys == "LINUX" && Memory >= 2000 && Arch
=="X86_64"
Output = out
Log = logfile
Error = ERR

Initialdir = d005
  Queue

Initialdir = d010
  Queue

Initialdir = d015
  Queue
```

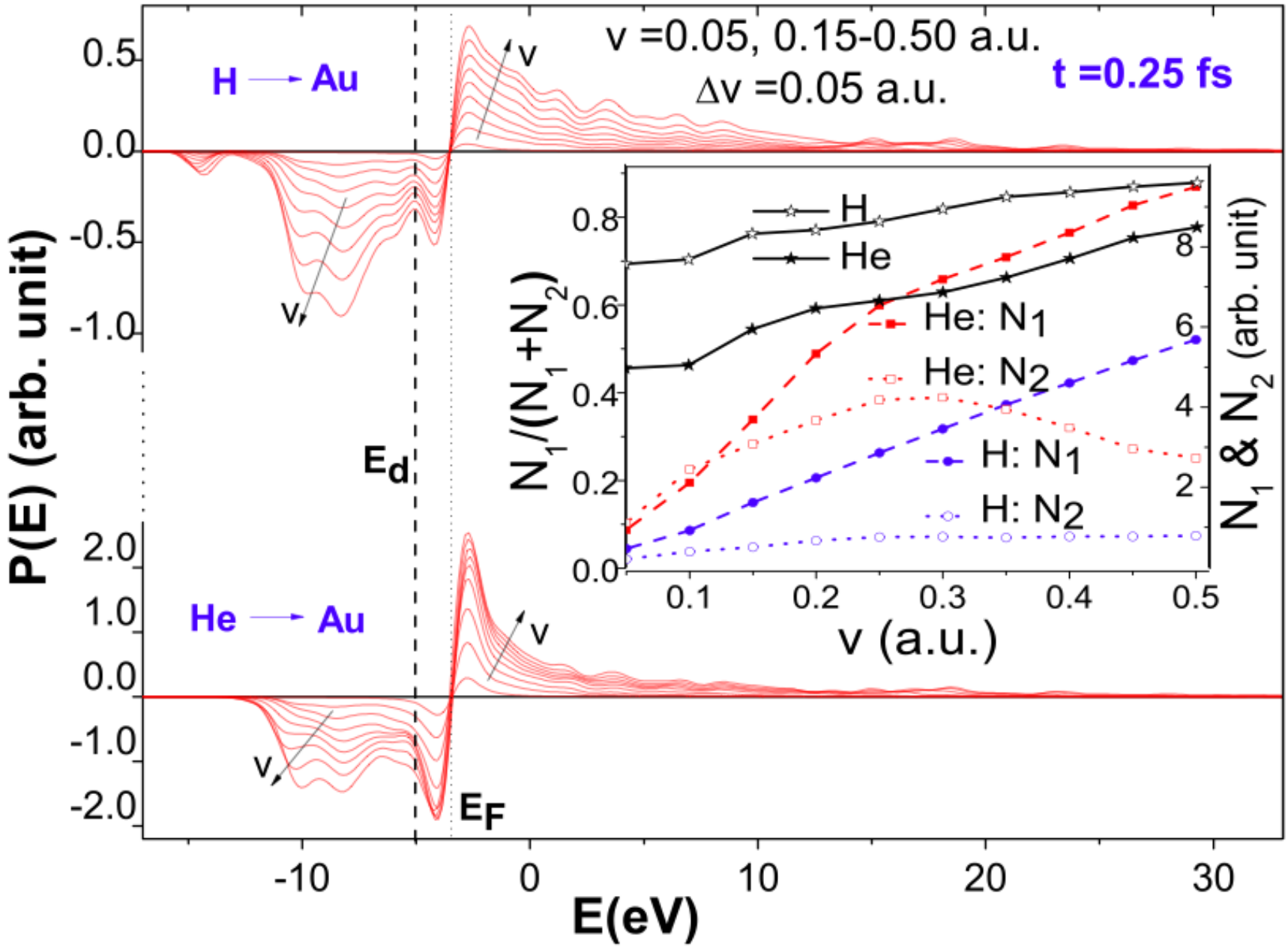
# Electronic distribution in adiabatic states

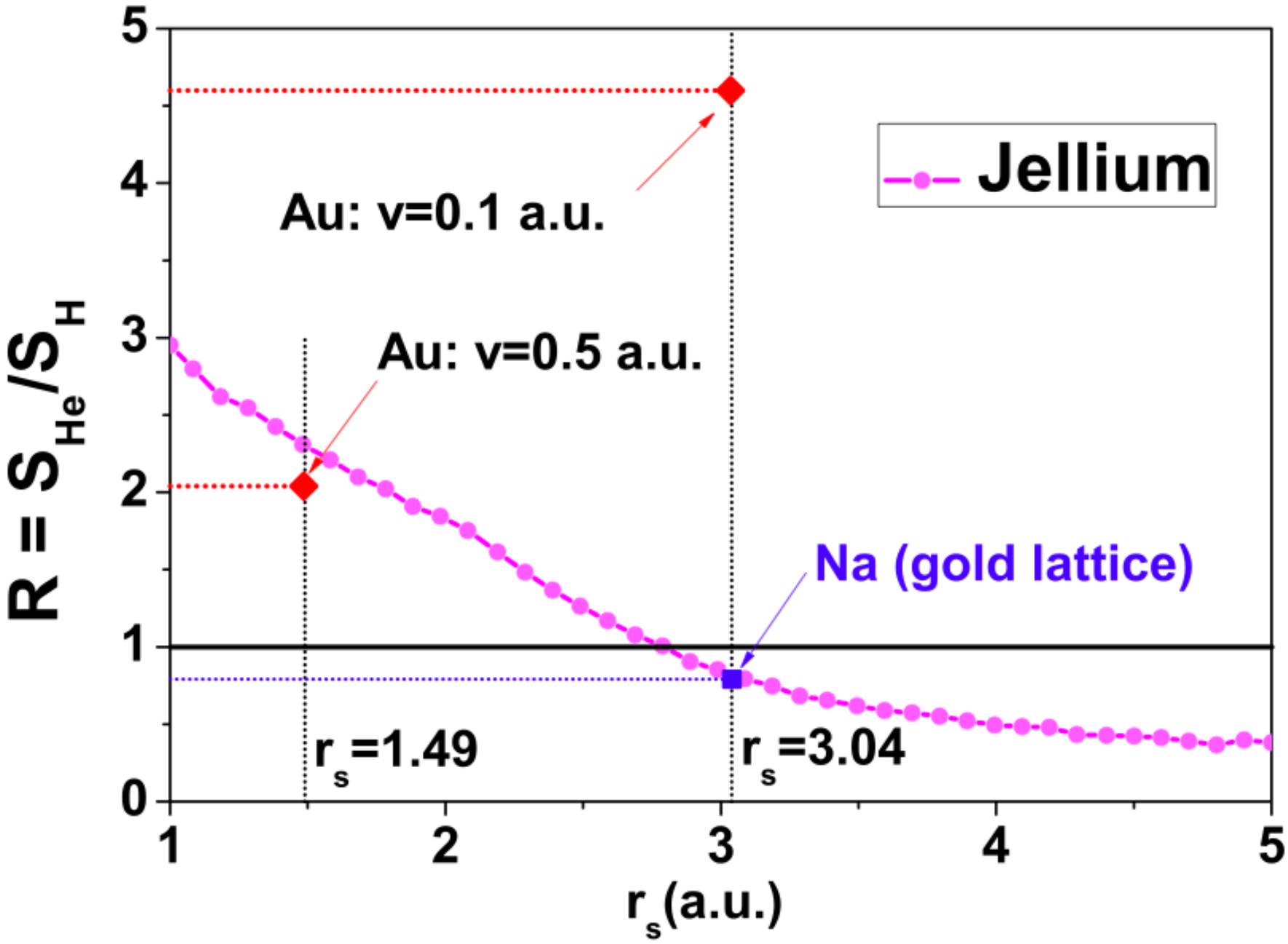
$$C_{ij} = \left\langle \Phi_i^{\mathbf{X}} | \Psi_j^{\mathbf{X}}(t) \right\rangle$$

$$O(E) = \sum_{i,j} |C_{ij}|^2 \delta(E - E_i)$$

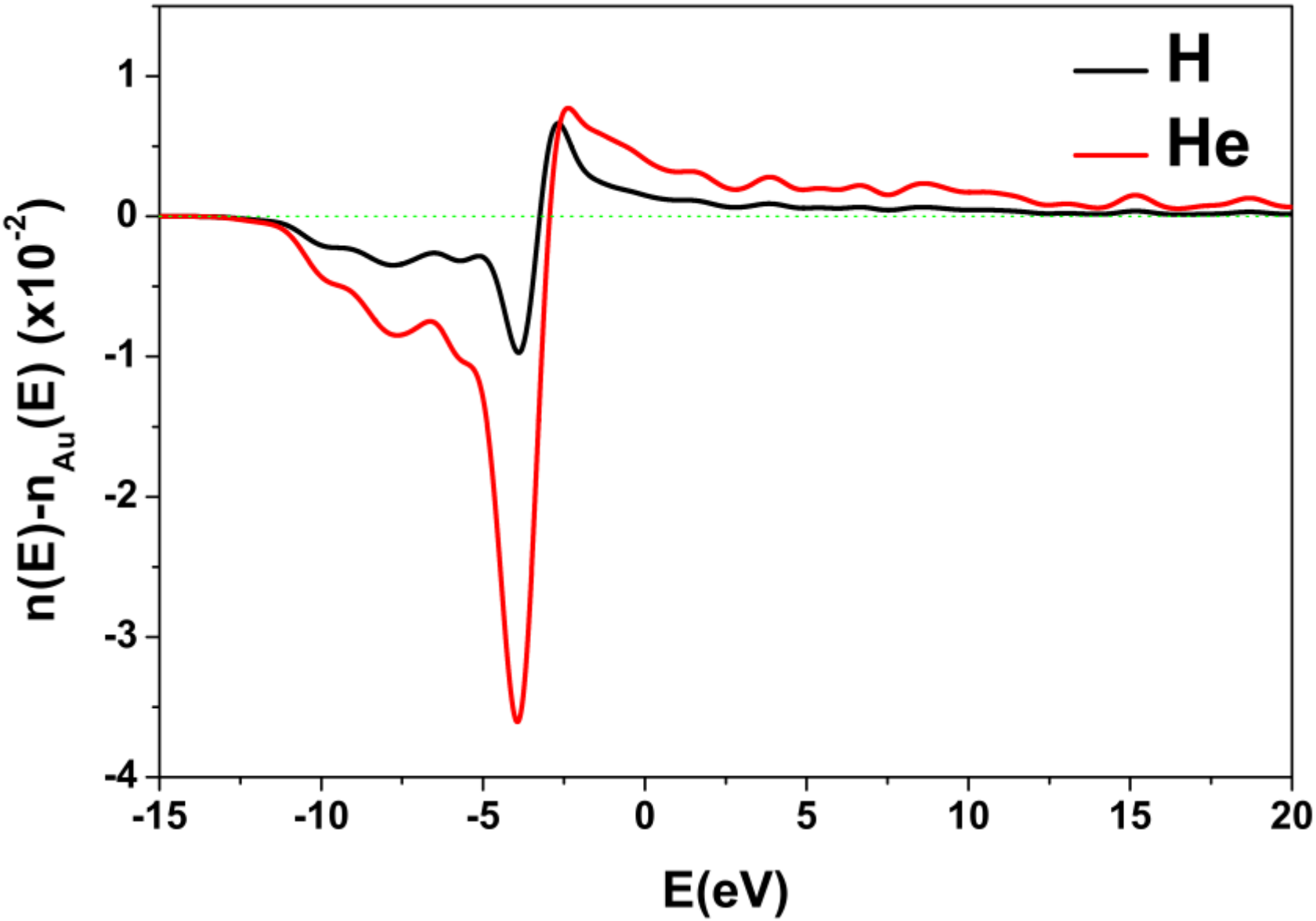
$$P(E) = O(E) - \Theta(E_F - E) g(E)$$


H ⟶ Au <100>
v =0.05 a.u.
t =0.1-1.1fs
Δt =0.1fs
g(E)
t
t
A short transient
E_F
P(E) (arb. unit)
E(eV)
1.0
0.5
0.0
-0.5
-1.0
-15
-10
-5
0
5


v =0.05, 0.15-0.50 a.u.
Δv =0.05 a.u.
t =0.25 fs
H → Au
He → Au
v
E_d
E_F
P(E) (arb. unit)
E(eV)
H
He
He: N1
He: N2
H: N1
H: N2
N1/(N1+N2)
N1 & N2 (arb. unit)
v (a.u.)


Jellium
Au: v=0.1 a.u.
Au: v=0.5 a.u.
Na (gold lattice)
$r_s$=1.49
$r_s$=3.04
$R = S_{He}/S_H$
$r_s$(a.u.)
0
1
2
3
4
5

Static impurity screening: a change in electronic distribution in adiabatic states without the impurity



# Summary & Conclusions

- We obtained a very good quantitative agreement with the experiments.

  Jellium picture does not fit on transition metals.

- Our method can be used to describe non-adiabatic processes in real materials.

Thanks!