Ab initio simulation of the formation of gold nanowires with impurities

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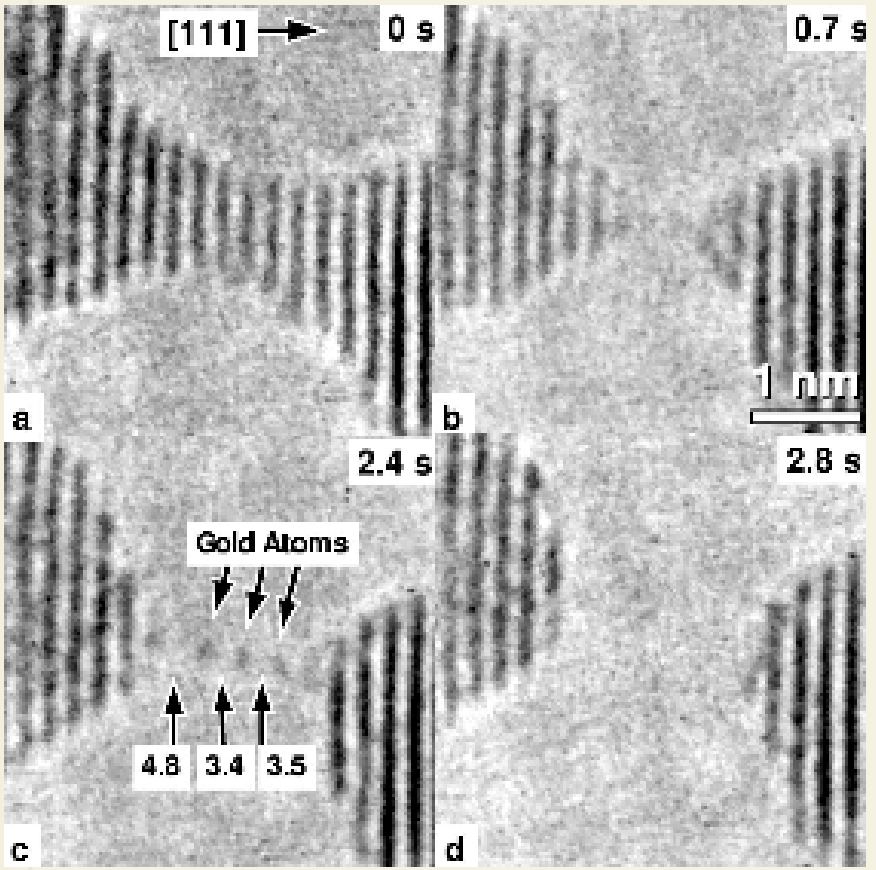
Gold nanowires



S. B. Legoas *et al.* Phys. Rev. Lett. **88,** 076105 (2002)

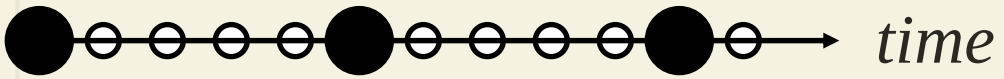
Accelerated dynamics

E. Anglada et al. PRB 66, 205101 (2002)

Double-force method

● Expensive force evaluations

○ Cheap force evaluations



Expensive forces:

- Kohn-Sham functional
- Converged basis set

Cheap forces:

- Harris functional
- Minimal basis set

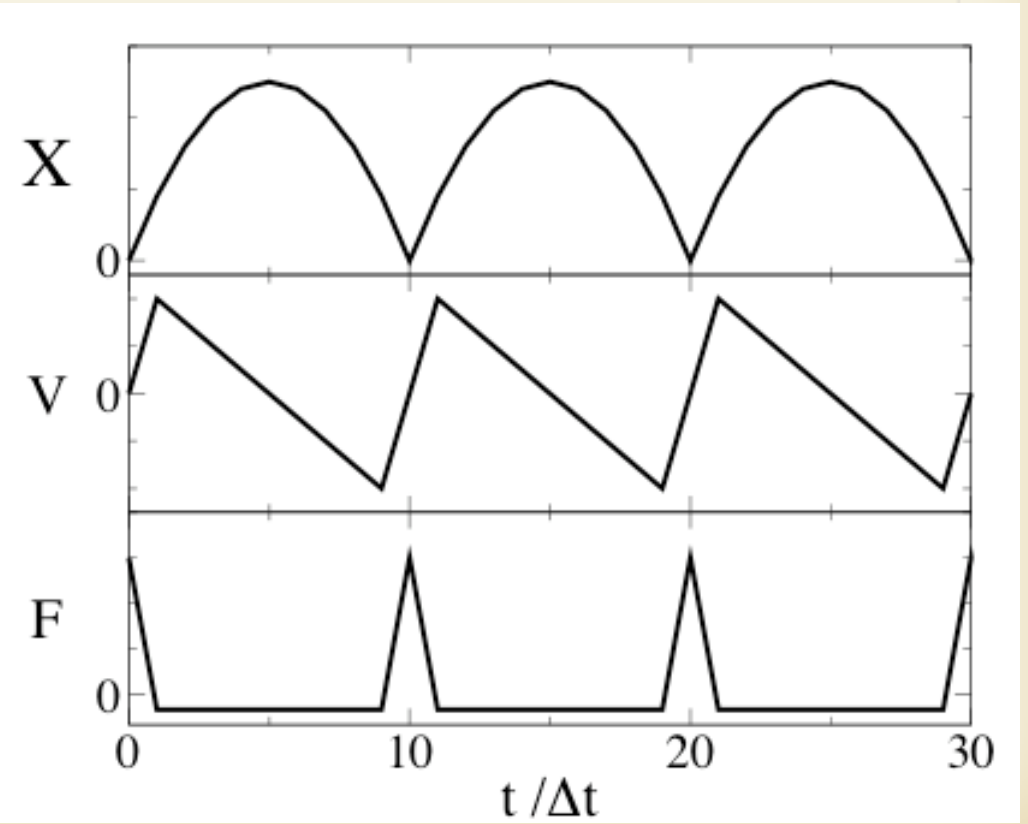
Example

$$x(0) = 0$$

$$v(0) = 0$$

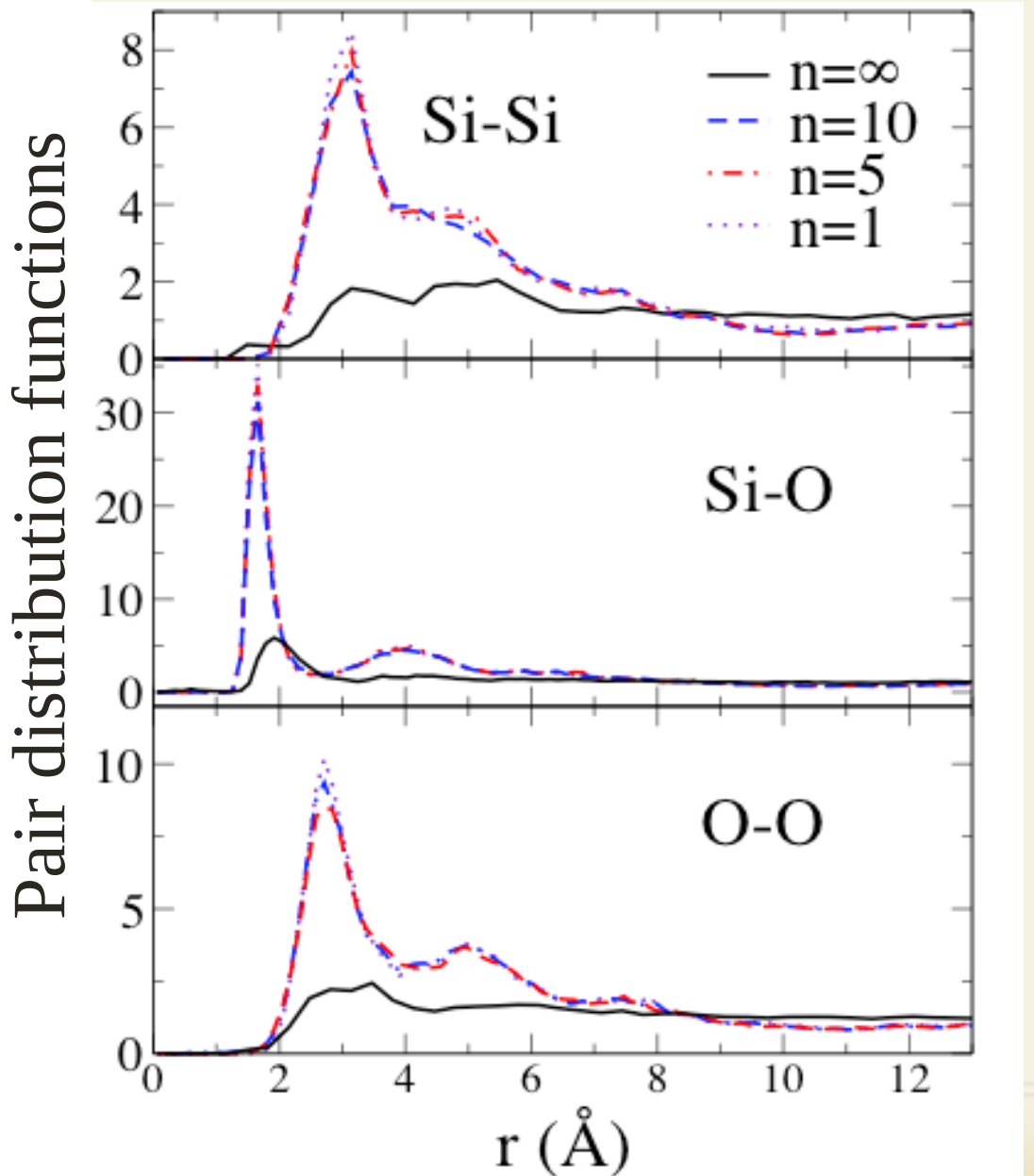
$$f_{expensive}(t) = 0$$

$$f_{cheap}(t) = -0.1$$



Accelerated simulations

SiO_2



$$n = \frac{\Delta t_{expensive}}{\Delta t_{cheap}}$$

72 atoms

5500 K

0.42 gr/cm^3

Wire-formation simulations

Initial geommetry:

Thick column of 50-150 atoms with **periodic** boundary conditions

Annealing at 2000 K for 3 ps

Impurity at **random** substitutional position

Further annealing for three more ps

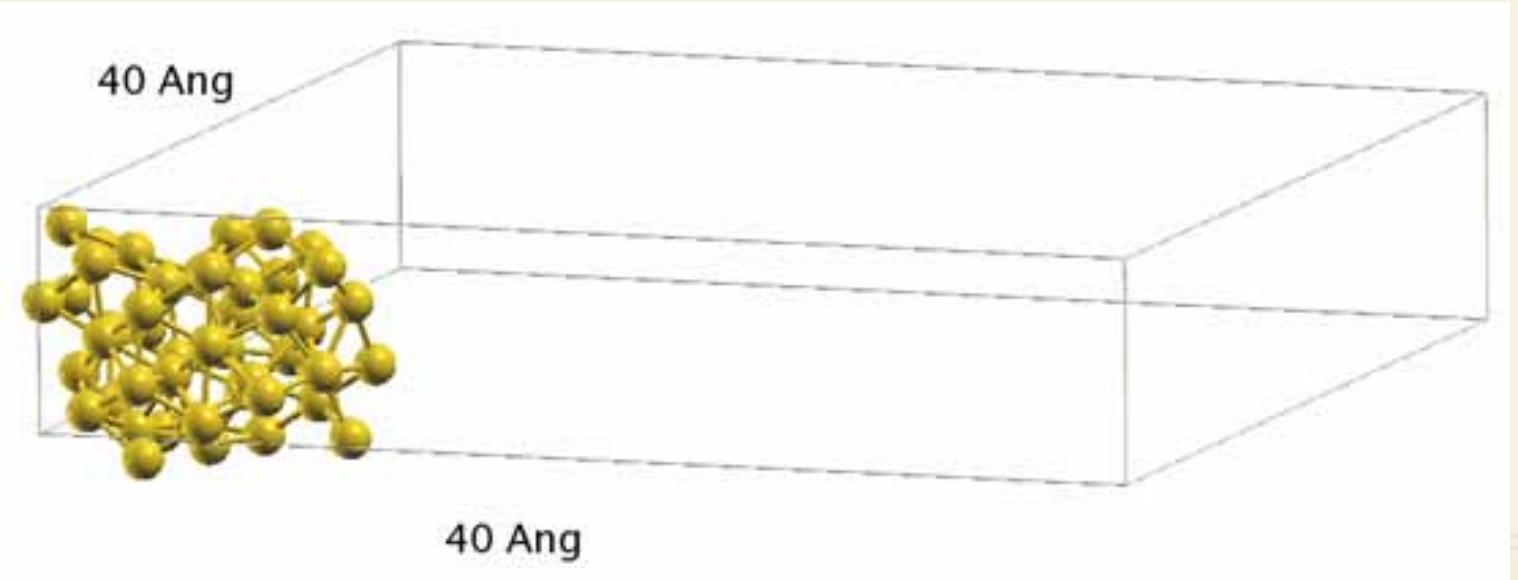
Quenching to 300 K

Wire stretching:

50-1000 K (most at 600 K)

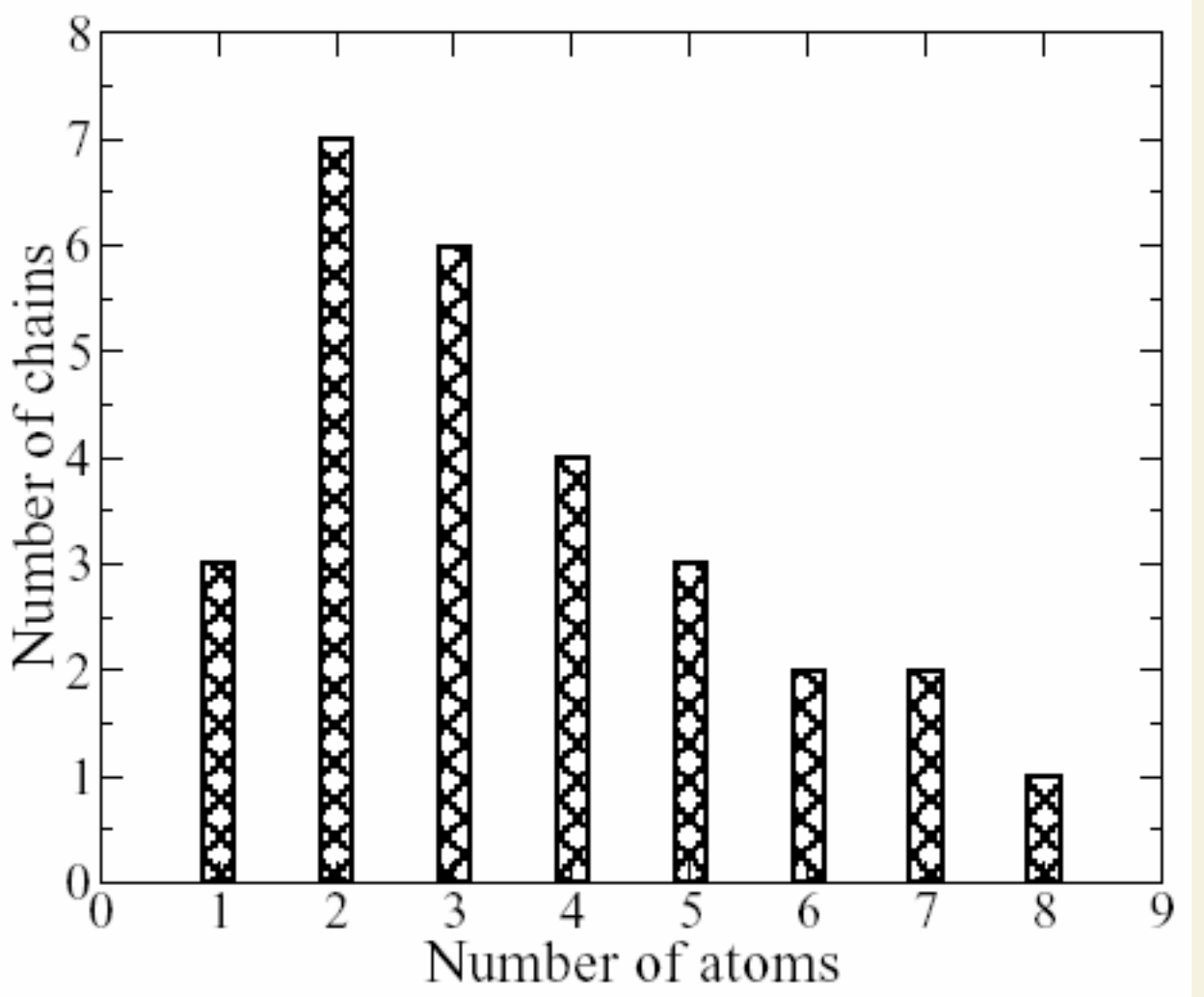
1-3% stretch every 100-300 fs

Velocities rescaled every 50 ps



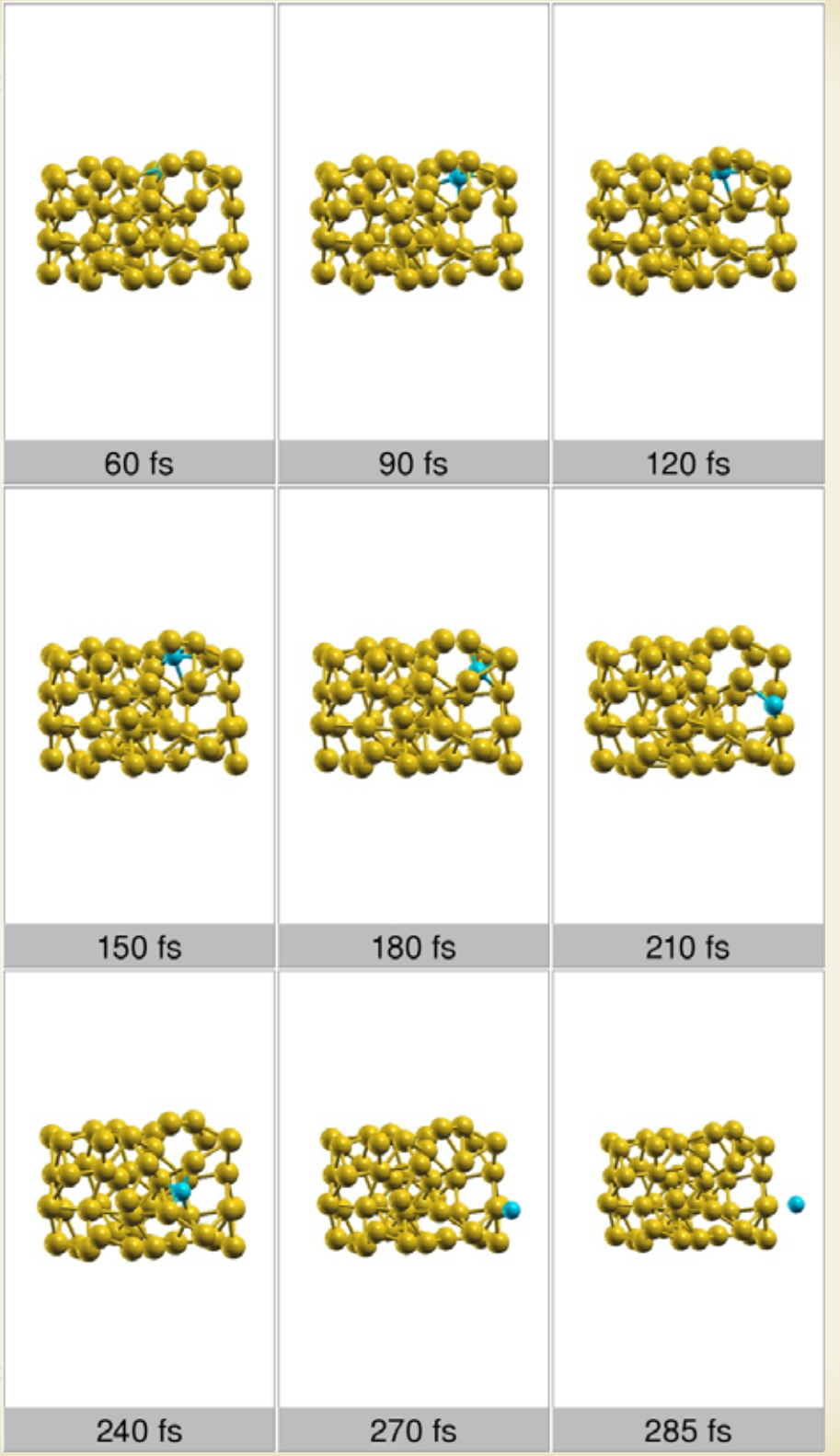
Pure-gold wires

25 simulations



Hydrogen

15 simulations →
0 times in the chain
(always evaporates)

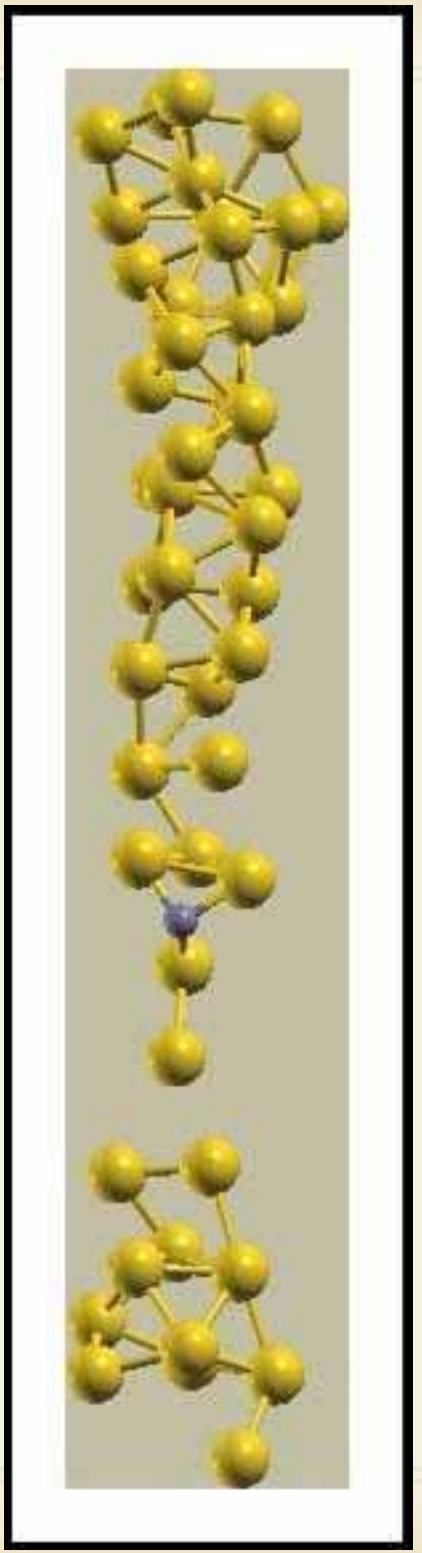


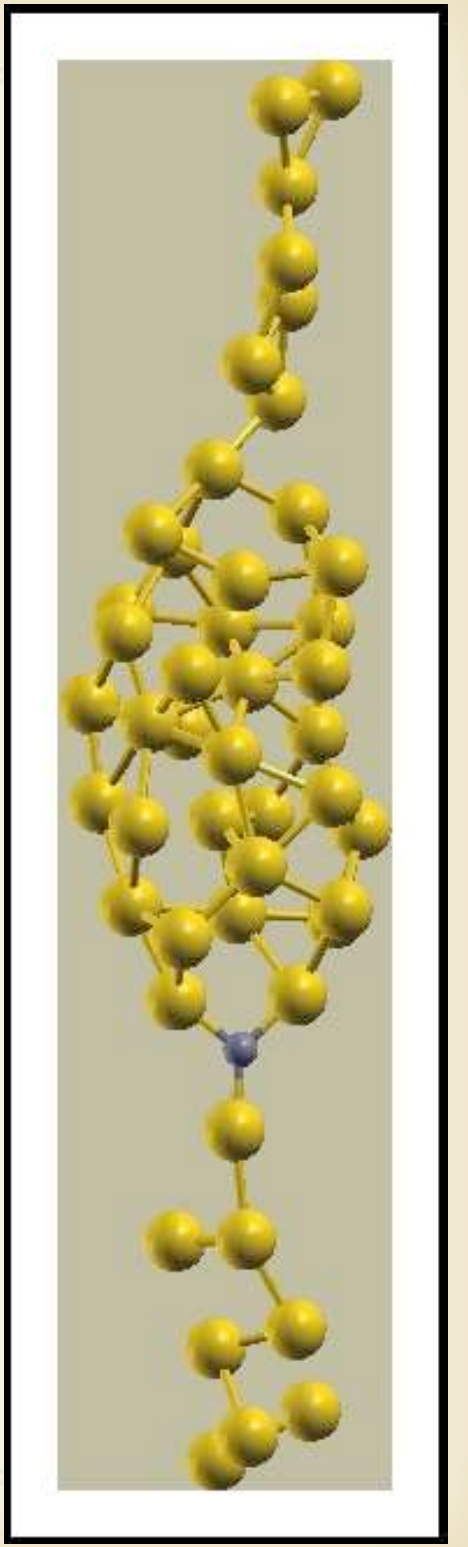
Carbon

10 simulations → 1 time
in the chain

Breaking force: 3.4 nN

Distance Au-C-Au: 3.1-3.4 Ang



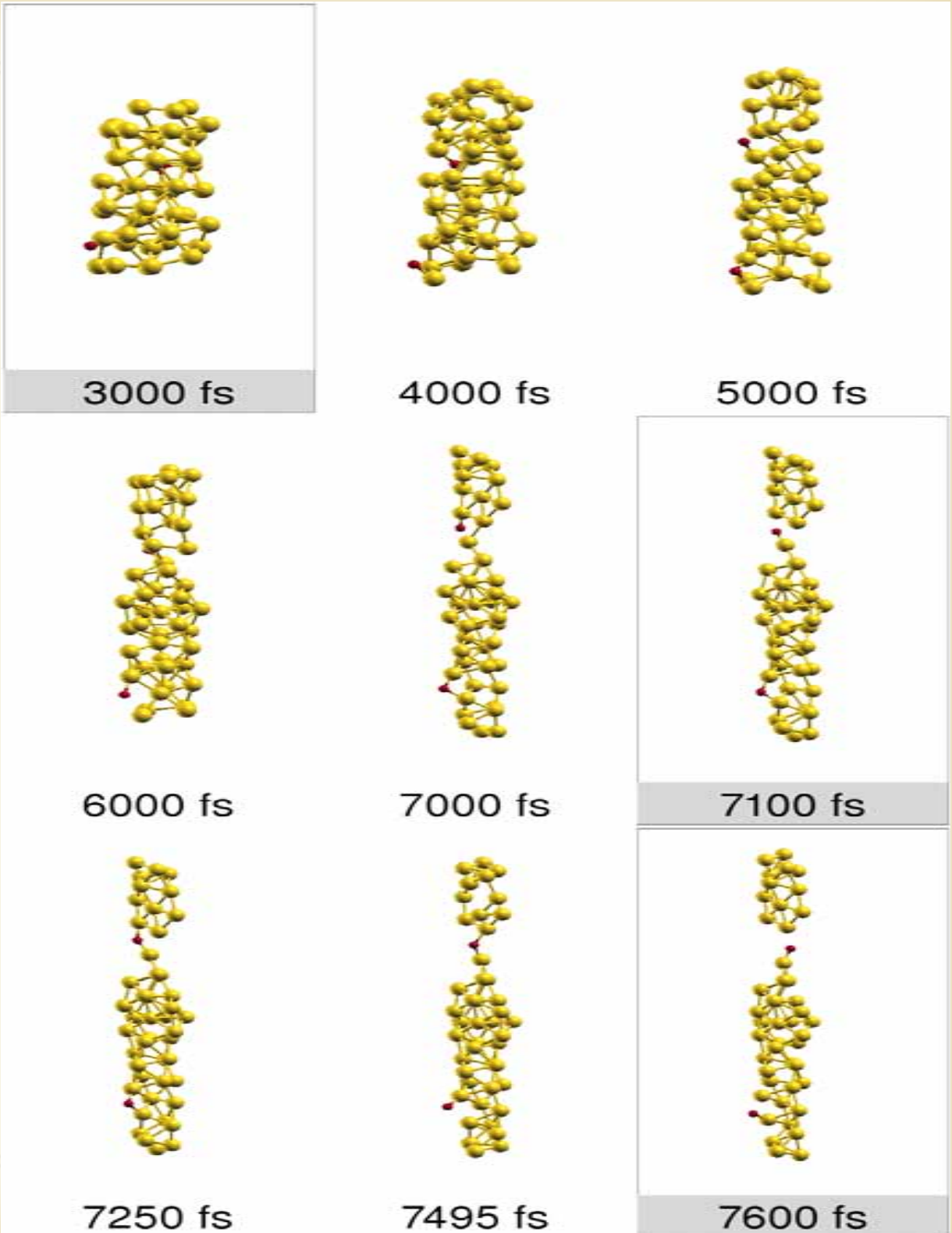


Oxygen

10 simulations →
1 time in the chain

Breaking force (LDA): 12 nN!

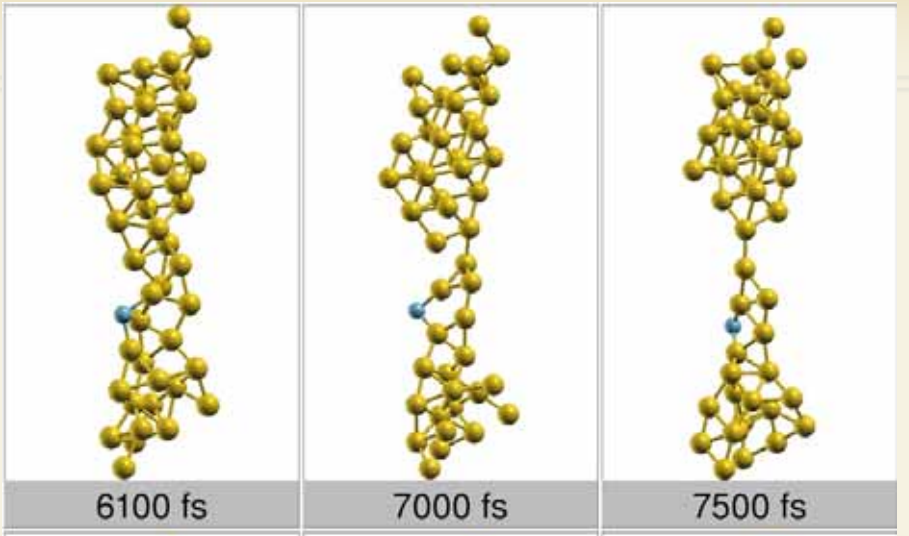
Distance Au-O-Au: 4.4 Ang

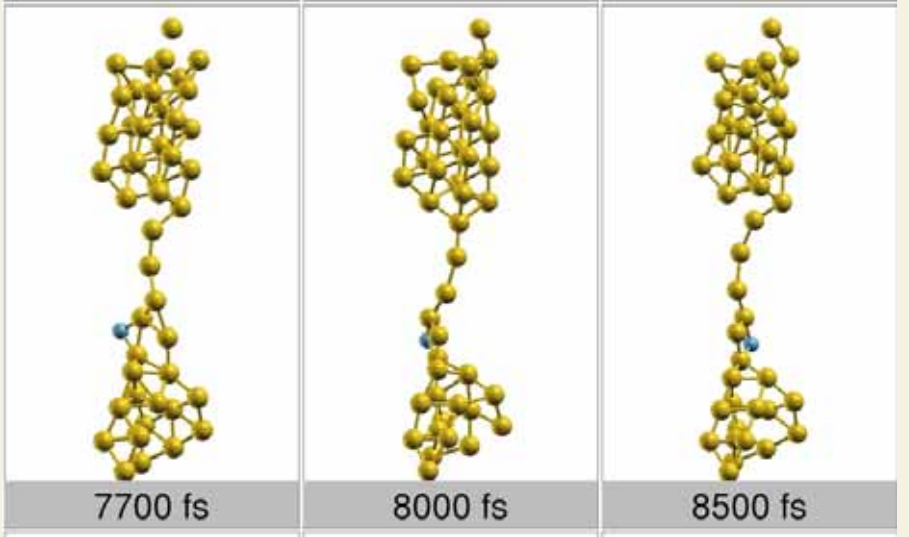


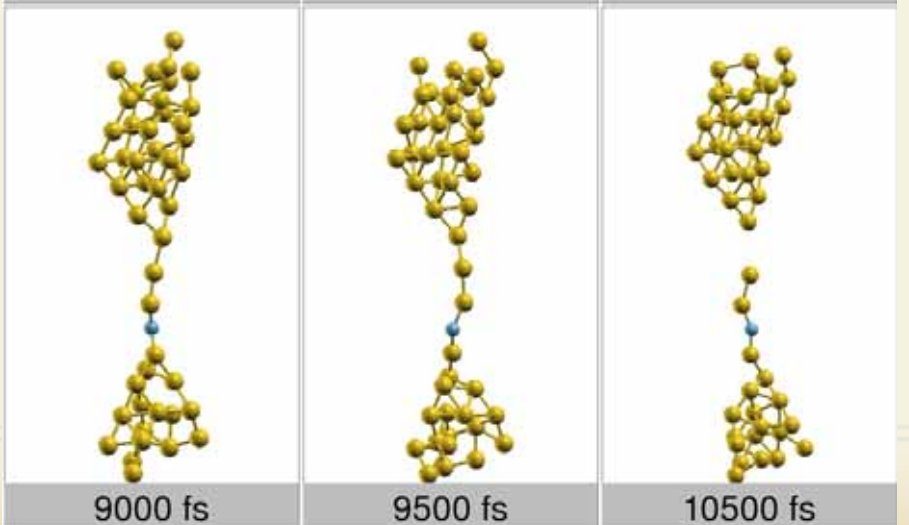
Sulphur

13 simulations
12 times in the chain

Breaking force: 2.5 nN
Distance Au-S-Au:
5.0 ± 0.2 Ang.



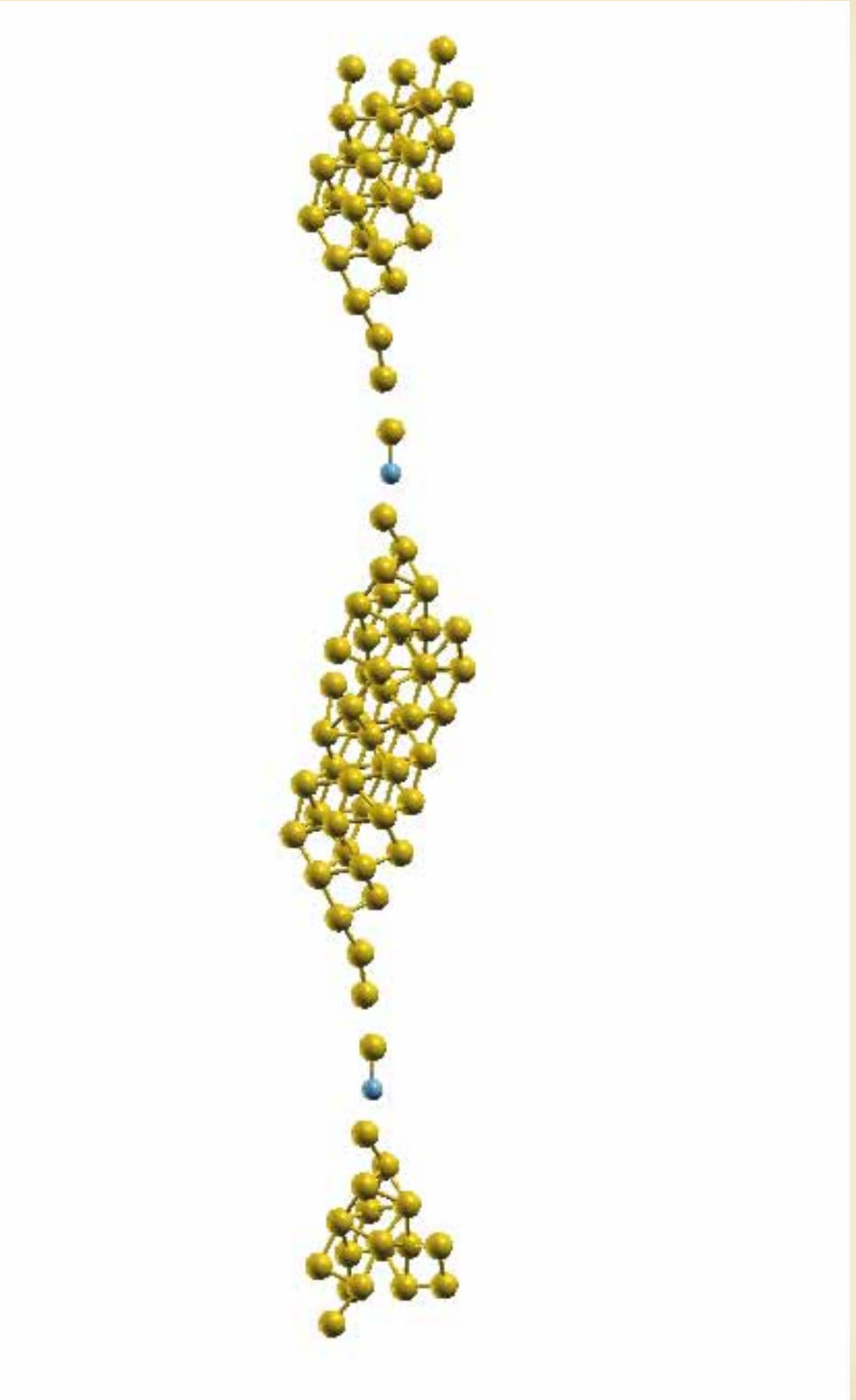




Giant monoatomic chain

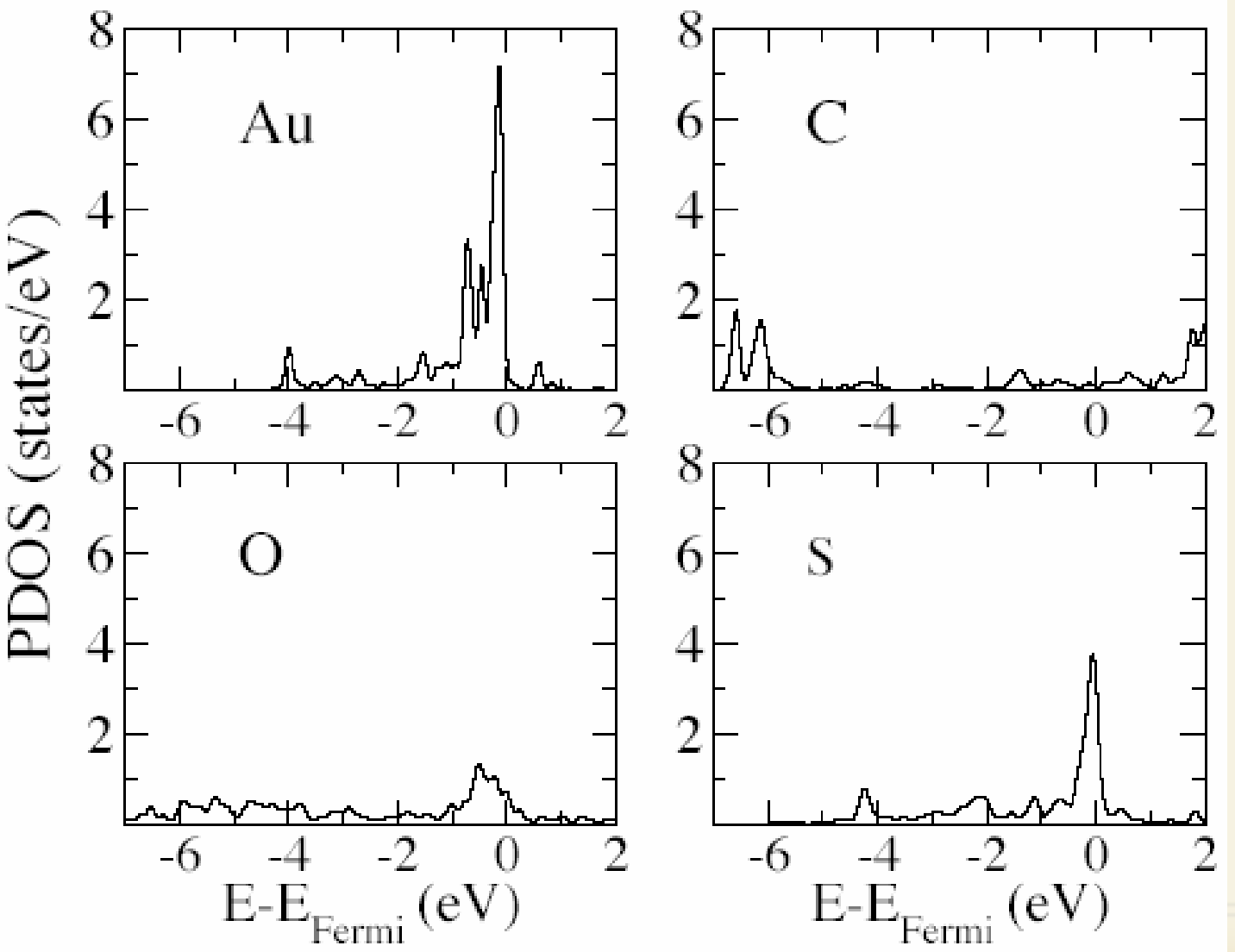
15 atoms long !!!

Two S impurities
→ two chains



Projected density of states

$$\rho_\alpha(\varepsilon) = \sum_i \left| \langle \alpha \mid \psi_i \rangle \right|^2 \delta(\varepsilon_i - \varepsilon)$$



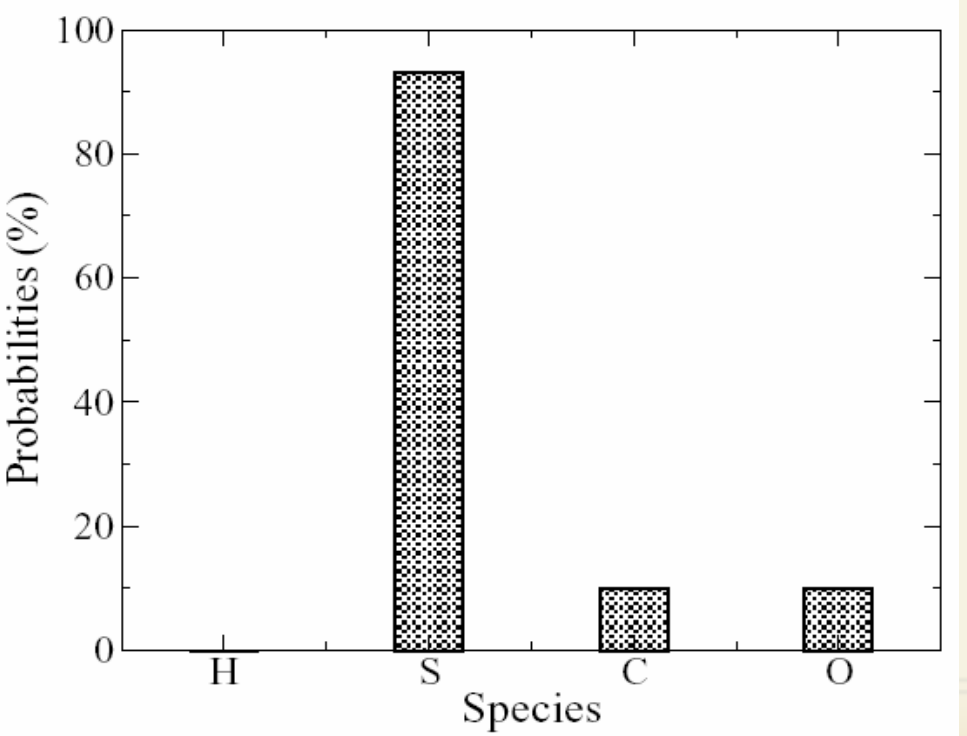
Au-X-Au distances

	Distance (Ang)
Au-Au	2.9 ± 0.2
Au-C-Au	3.3 ± 0.2
Au-O-Au	4.4 ± 0.1
Au-S-Au	5.0 ± 0.2

Account for all experimental distances

Conclusions

- Sulphur likes to be in monoatomic gold wires
- Carbon and oxigen also have a small probability
- Au-Au distances in good agreement with experiments
- Sulphur has a large PDOS at E_F



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