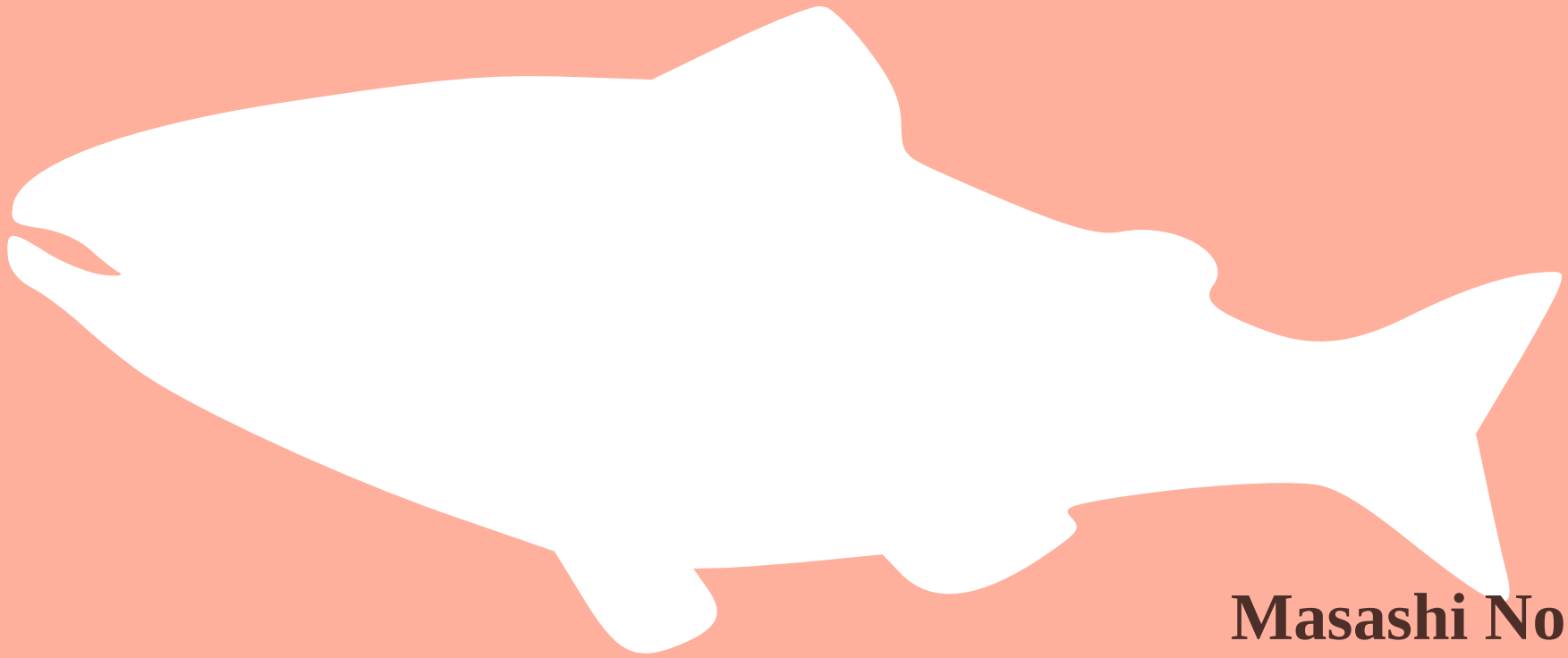
How to Use SALMON-1: Isolated Systems

Overview



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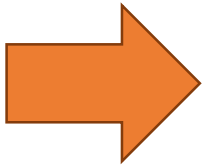
Flowchart and equations for isolated systems

GS (Ground State) calculation (determination of initial states)



RT (Real-time) calculation (propagation of states)

- Ground state calculation

$$\left\{-\frac{1}{2}\nabla^2 + V_{ion} + V_H + V_{xc}\right\}\psi_n(\boldsymbol{r}) = \epsilon_n\psi_n(\boldsymbol{r})$$

ψ_n: Kohn-Sham orbital

ϵ_n: 1-particle energy

V_{ion}: Electron-nuclear interaction potential

V_H: Hartree potential

V_{xc}: Exchange-correlation potential

- Time evolution calculation

$$i\hbar\frac{\partial}{\partial t}\psi_n(\boldsymbol{r},t) = \left\{-\frac{1}{2}\nabla^2 + V_{ext}(\boldsymbol{r},t) + V_{ion} + V_H + V_{xc}\right\}\psi_n(\boldsymbol{r},t)$$

$V_{ext}(\boldsymbol{r},t)$: External scalar potential

Optical response calculation

- Impulsive force

$$V_{ext}(t) = V_0\delta(t)$$

- Dipole moment

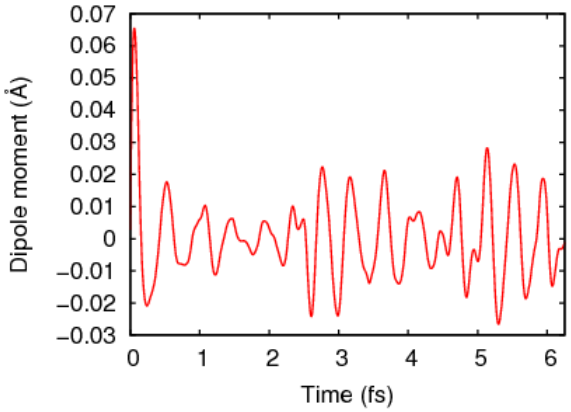
$$d(t) = -e\int r_v\big(\rho(\boldsymbol{r},t) - \rho(\boldsymbol{r},0)\big)d\boldsymbol{r}$$

- Oscillator strength function

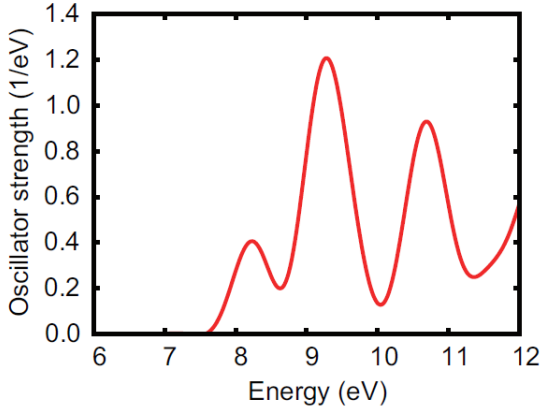
$$\frac{df_v(E)}{dE} = \frac{2mE}{\pi\hbar^3}\,\mathrm{Im}\int_0^T f\left(\frac{t}{T}\right)d(t)e^{iEt/\hbar}dt$$

C_2H_2 molecule

- Dipole moment



- Oscillator strength function



Pulse calculation

- External field

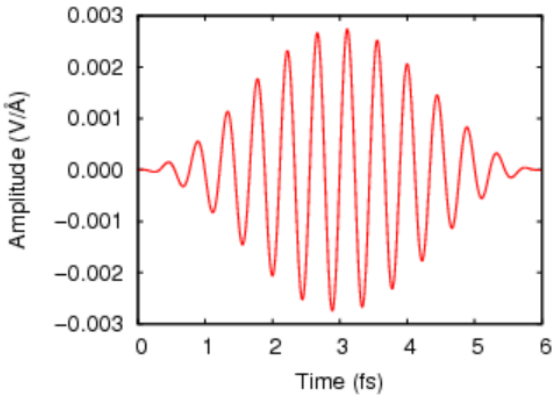
$$V_{ext}(t) = E_0 \cos^2\left(\frac{\pi(t-t_0)}{T}\right)\cos(\omega t + \phi)$$

- Dipole moment

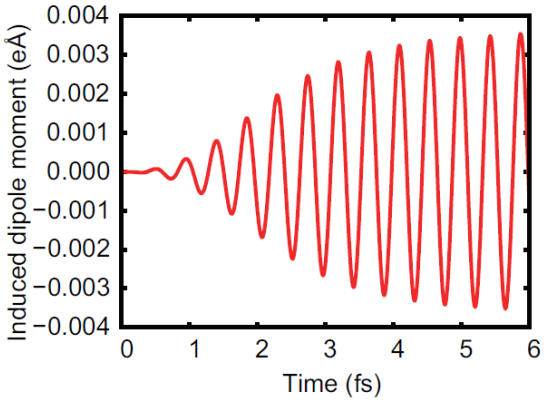
$$d(t) = -e\int r_v\big(\rho(\boldsymbol{r},t) - \rho(\boldsymbol{r},0)\big)d\boldsymbol{r}$$

The C_2H_2 molecule under a laser pulse ($\omega = 9.28$eV)

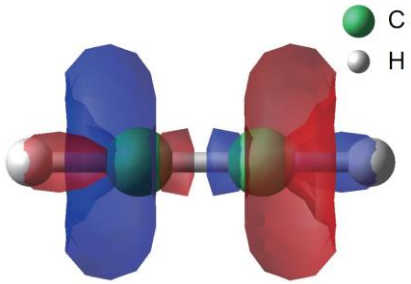
- Shape of pulse



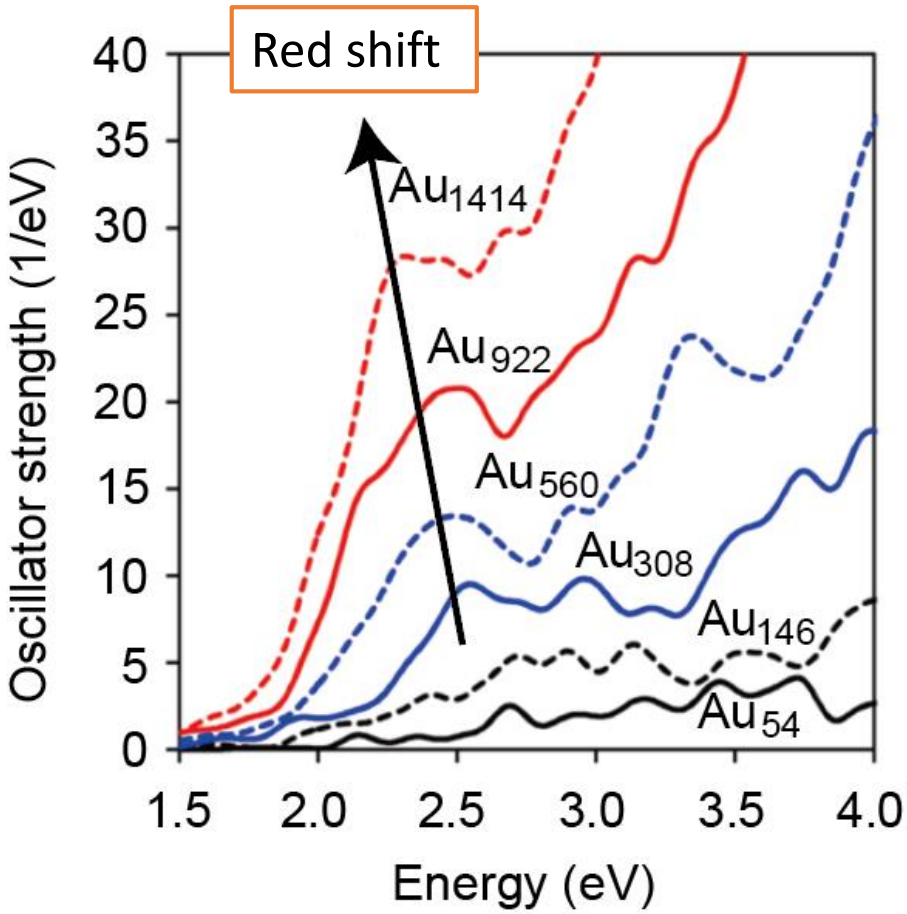
- Dipole moment



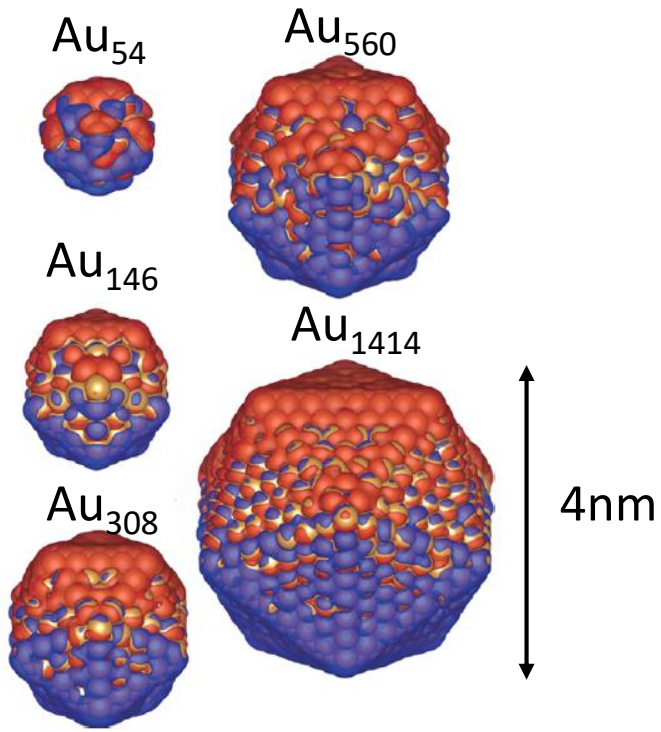
- Difference of electron density



Applications (1): gold nanocluster



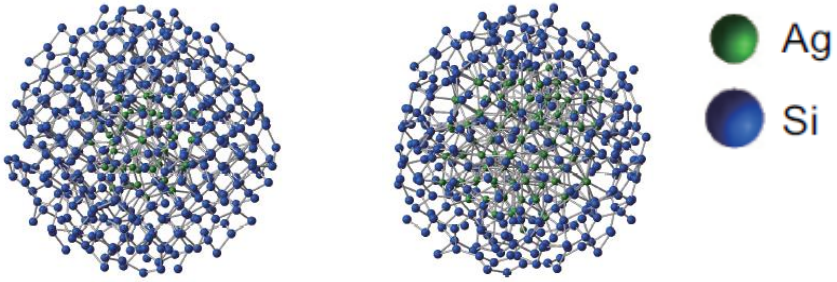
Difference of electron density



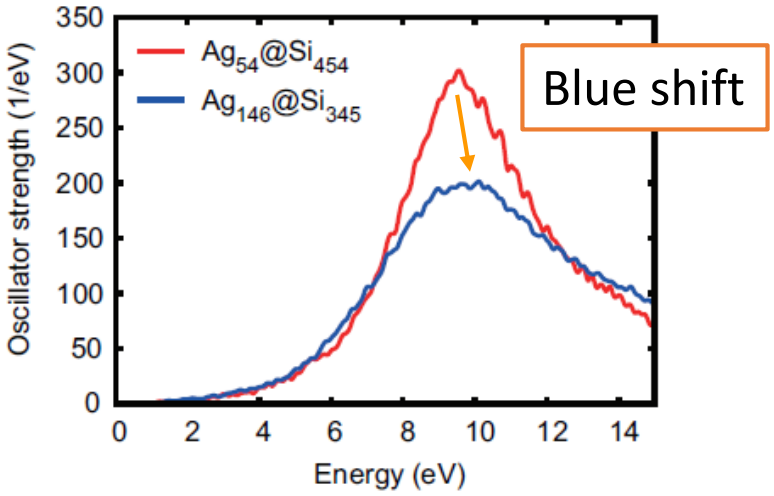
Localized surface plasmon resonance gradually grows with increasing cluster size.

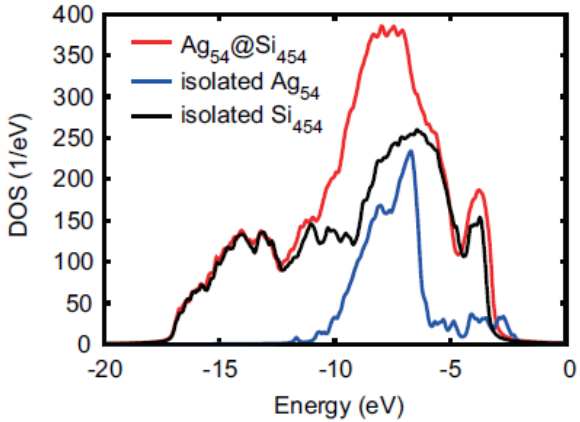
Applications (2): coreshell structures

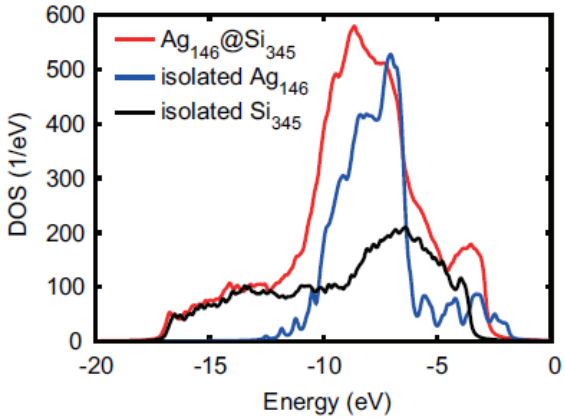
$Ag_{54}@Si_{454}$ $Ag_{146}@Si_{345}$



Diameter: 2.5nm







DOS of coreshell structures differs