OPTICAL PROPERTIES OF METALLIC NANOPARTICLES, MOLECULES AND POLYMERS

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Mie Theory -
Dilute Colloidal
Solution Limit

Spherical Particles

Ref: C. F.Bohren and D. R. Huffman, Absorption and Scattering of Light by Small Particles, Wiley: New York, 1983.

Extinction Cross-section of Spherical Particles

$$C_{ext} = \frac{24\pi^2 R_p^3 \varepsilon_m^{3/2}}{\lambda} \frac{\varepsilon_p''}{\left(\varepsilon_p' + 2\varepsilon_m\right)^2 + \varepsilon_p''^2}$$

ε_m – Dielectric Function of the Medium

R_p - Particle Radius

λ - Incident Wavelength

ε'_p – Real Part of Dielectric Function of Particles

ε''_p – Imaginary Part of Dielectric Function of Particles

Dielectric Function of the Nanoparticles

$$\varepsilon_p = \varepsilon'_p + i\varepsilon''_p$$

Complex Dielectric Function For Bulk Material

$$\varepsilon_{bulk}(\omega) = 1 - \frac{\omega_P^2}{m_e(\omega^2 + i\omega\Gamma)} = \varepsilon'_{bulk}(\varepsilon) + i\varepsilon''_{bulk}(\varepsilon)$$

m_e – Mass of Electron

ω – Excitation Angular Frequency

$$\omega_P = ne^2 / m_e \varepsilon_0$$

Bulk Plasmon Frequency

e – **Electron Charge**

n – **Density of Free Electrons**

ε_0 – **Permittivity of Free Space**

$$\Gamma = \frac{v_F}{l_e} = \frac{1}{\tau}$$

Damping Frequency

v_F – **Fermi Velocity**

l_e – **Mean Free Path**

τ – **Relaxation Time**

Real Part of Dielectric Function of Bulk Material

$$\varepsilon'_{bulk}(\omega) = 1 - \frac{\omega_P^2}{\omega^2 + \Gamma^2}$$

Imaginary Part of Dielectric Function of Bulk Material

$$\varepsilon''_{bulk}(\omega) = \frac{\omega_P^2 \Gamma}{\omega\left(\omega^2 + \Gamma^2\right)}$$

Corrected Real Part of Dielectric Function of Bulk Material

$$\varepsilon'_{bulk}(\omega) = \varepsilon_\infty - \frac{\omega_P^2}{\omega^2 + \Gamma^2}$$

ε_∞ - High Frequency Dielectric Constant

Effect of the Small Particle Size

Particle Size Effective Mean-Free Path

$$\frac{1}{l_{eff}} = \frac{1}{l_e} + \frac{1}{R_p}$$

Effective Damping Frequency

$$\Gamma_{eff} = \frac{v_F}{l_{eff}}$$

Effect of Intrabound Transitions

Free-electron Real Part of the Dielectric Function of Spherical Particles

$$\varepsilon'_p(\omega) = \varepsilon_\infty - \frac{\omega_P^2}{\omega^2 + \Gamma_{eff}^2}$$

Free-electron Imaginary Part of the Dielectric Function of Spherical Particles

$$\varepsilon''_p(\omega) = \frac{\omega_P^2 \Gamma_{eff}}{\omega\left(\omega^2 + \Gamma_{eff}^2\right)}$$

Total Complex Dielectric Function

$$\varepsilon_i(\omega) = \varepsilon_i^{free}(\omega) + \varepsilon_i^{interband}(\omega) \qquad (i = bulk, p)$$

Dielectric Constant in Metallic Nanoparticles

$$\varepsilon_p(\omega) = \varepsilon_p^{free}(\omega) + \varepsilon_{bulk}(\omega) - \varepsilon_{bulk}^{free}(\omega)$$

Dilute-dispersion Limit Adsorption Coefficient

$$\alpha_{ddl} = C_{ext}\rho_N$$

ρ_N - Number Density of Particles

Non-spherical Particles

Ref: R. Gans, Ann. Phys., 47 (1915) 270

Extinction Cross Section of Non-Spherical Particles

$$C_{ext} = \frac{8\pi^2 R^3 \varepsilon_m^{3/2}}{3\lambda} \sum_j \frac{\left(1/P_j^2\right)\varepsilon_p''}{\left(\varepsilon_p' + \frac{1-P_j}{P_j}\varepsilon_m\right)^2 + \varepsilon_p''^2} \qquad j = a,b,c$$

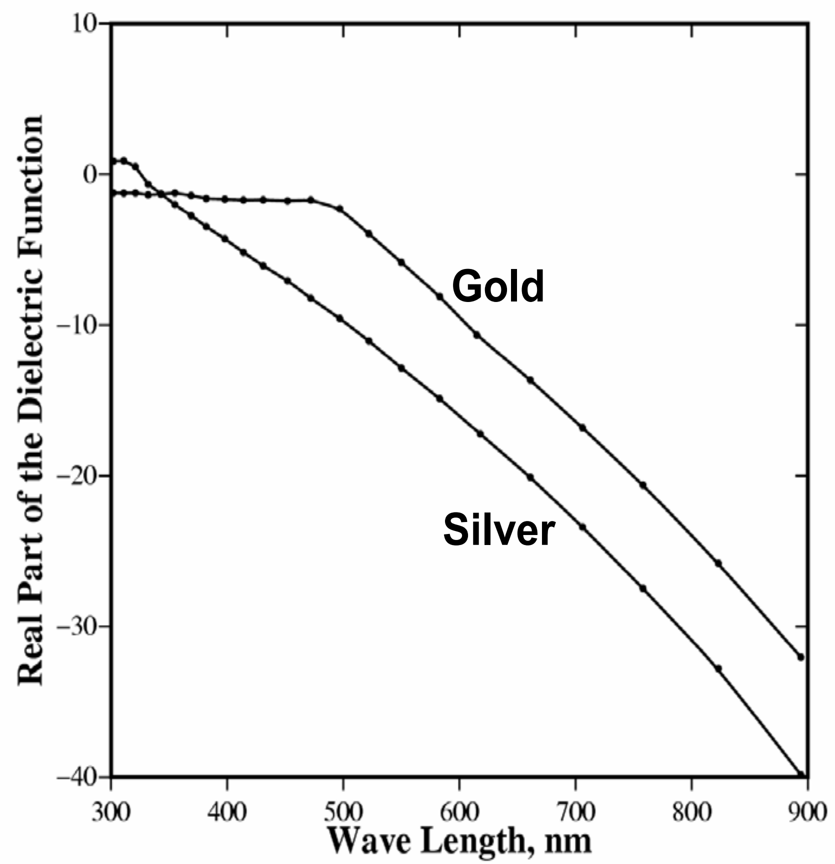
Depolarization Vector for Nanorod (a>b=c)

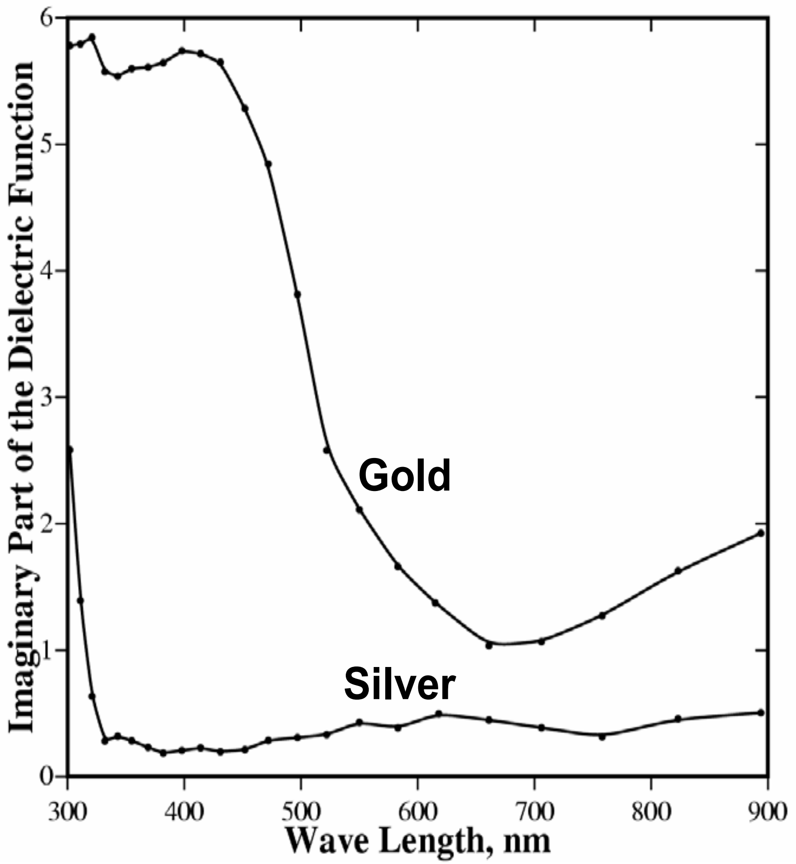
$$P_a = \frac{1-r^2}{r^2}\left[\frac{1}{2r}\ln\left(\frac{1+r}{1-r}\right) - 1\right]; \qquad P_b = P_c = \frac{1-P_a}{2}$$

where

$$r = \sqrt{1-\left(b/a\right)^2}$$

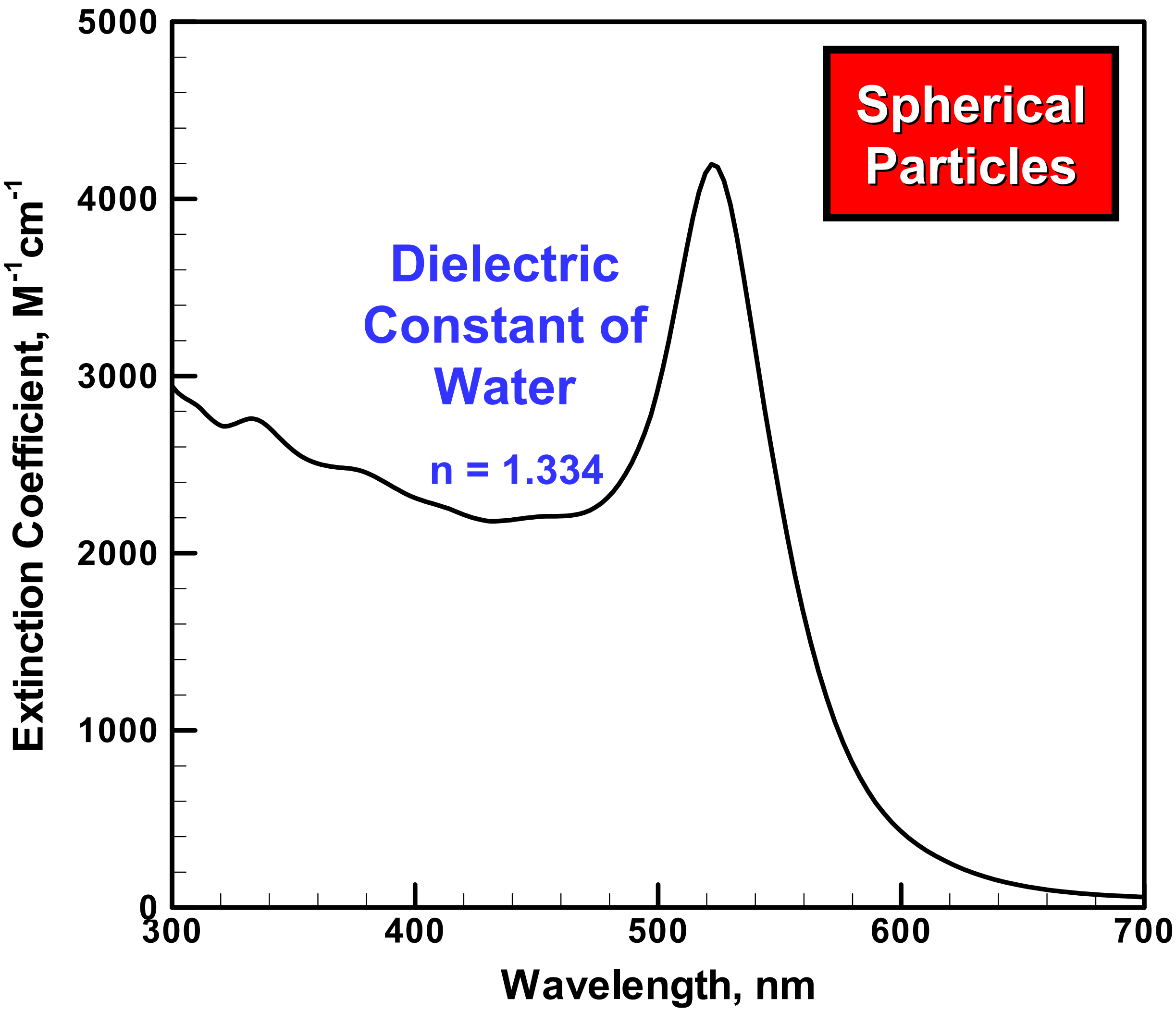
Input: Real and Imaginary Parts of the Dielectric Constants For Gold and Silver as a Function of the Photon Wavelength 4370



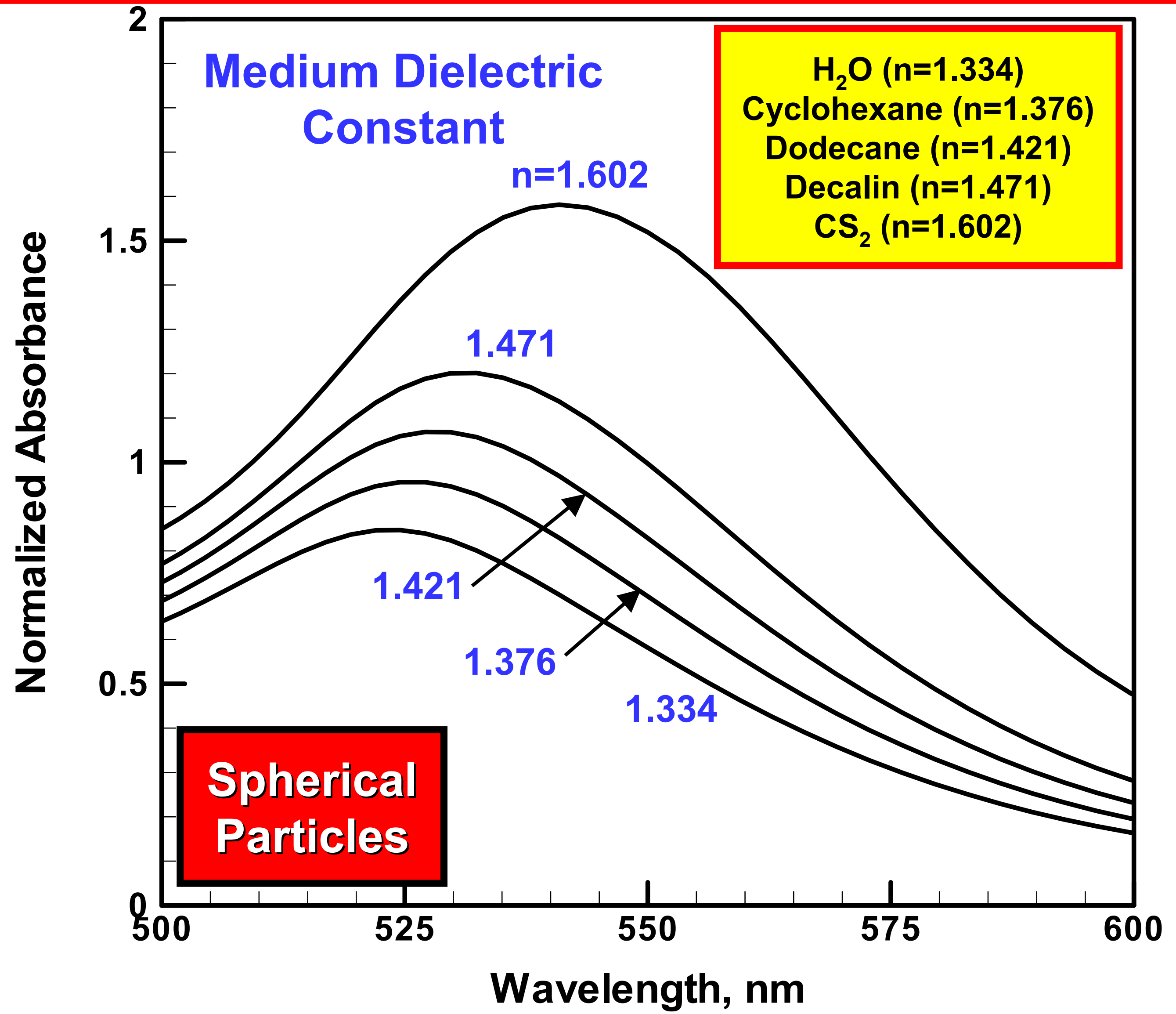


Ref: P. B. Johnson and R. W. Christy, Phys. Rev. B, 6 (1972) 4370

Results



Calculated Absorption Spectra of Au Particles in Water



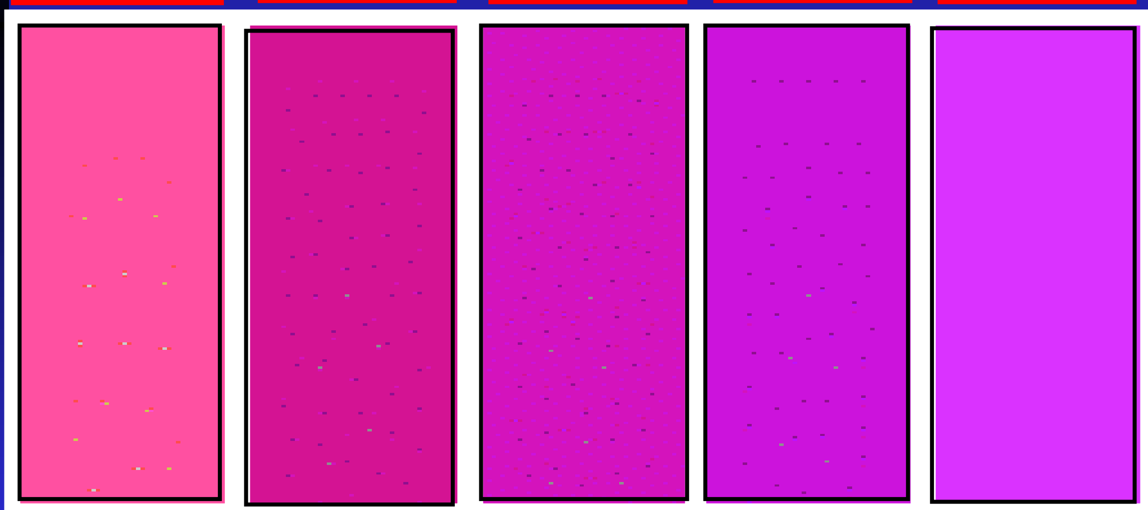
Calculated Absorption Spectra of Au Particles Media with DifferentDielectric Constant

Spherical Gold Particles
Effect of Dielectric Constant of the Medium

Experiment

n=1.334 | n=1.407 | n=1.481 | n=1.525 | n=1.583

Theory

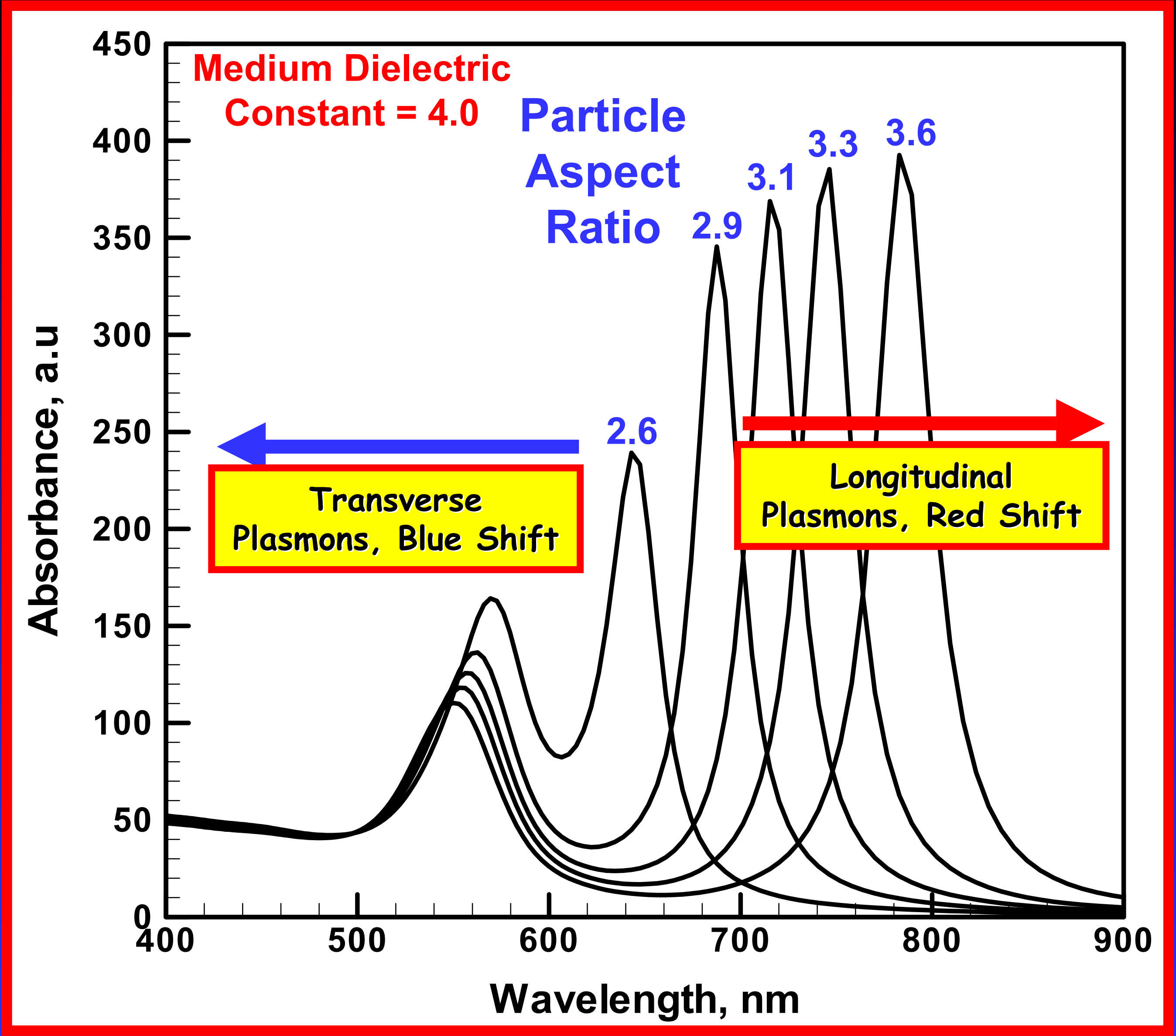


15 nm Au Spherical Particles in Water and in Mixtures of Butyl Acetate and Carbon Disulfide

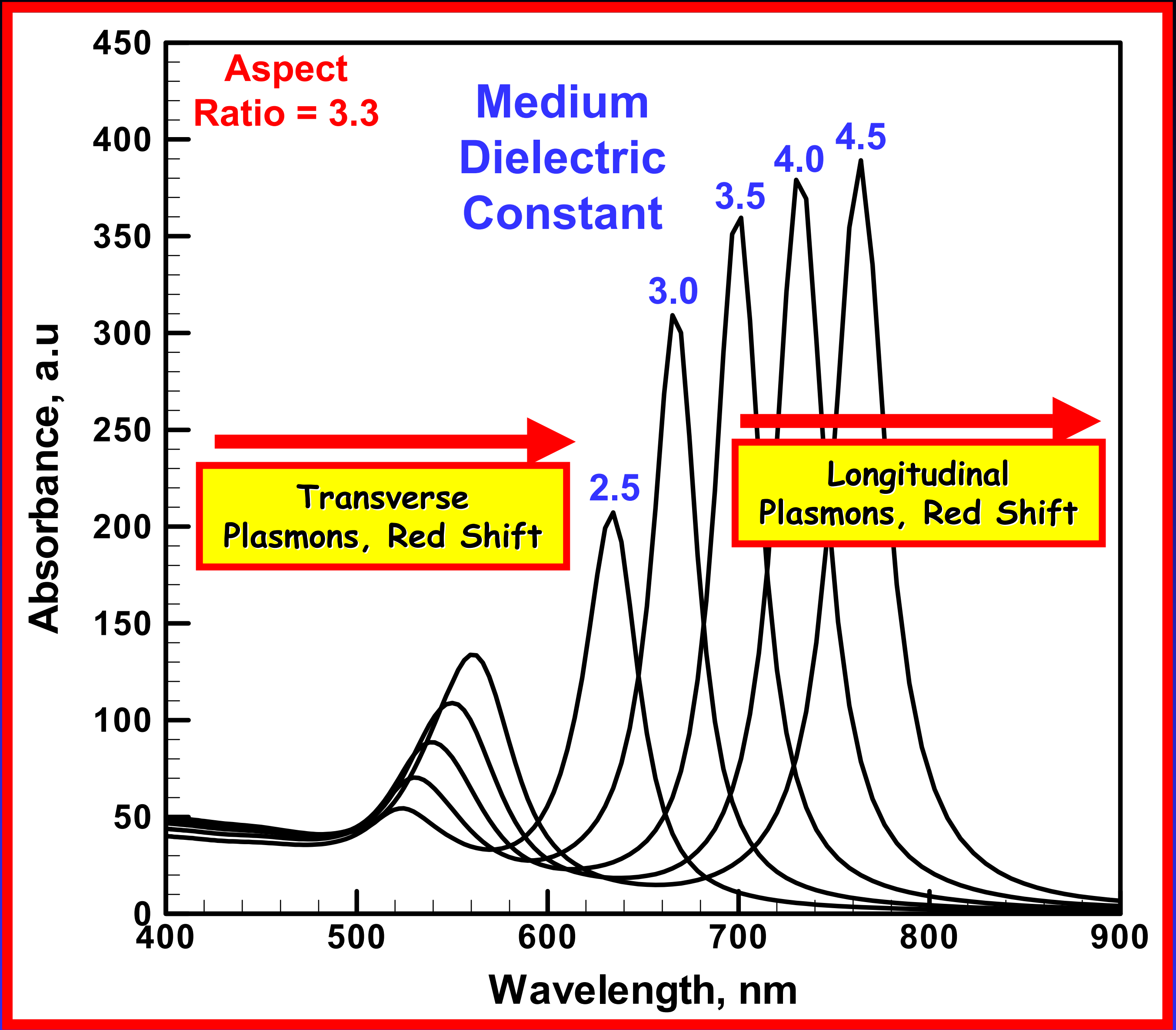
Ref: S. Underwood and P. Mulvaney, Langmuir, 10 (1994) 3427-3430

Spherical Particles

Mie Theory Transmission Colors



Elongated Ellipsoidal Particles



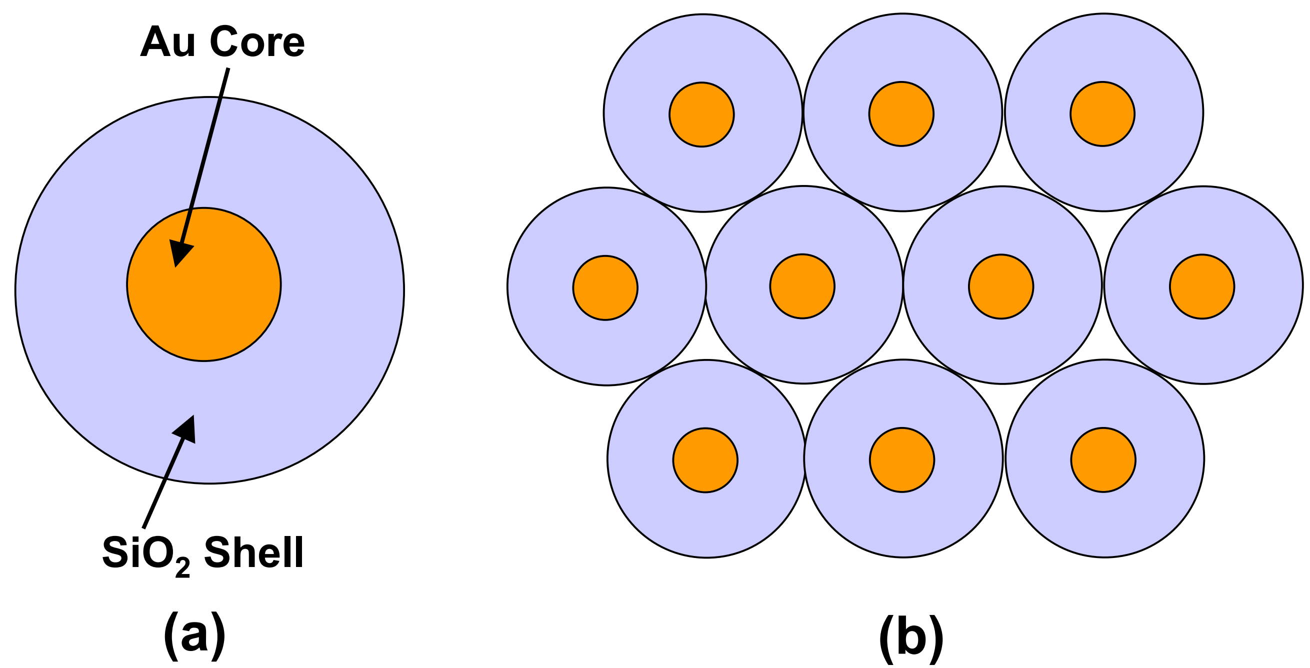
Elongated Ellipsoidal Particles

Regression Analysis of the Wavelength at the Longitudinal Plasmon Peak

$$\lambda_{\max} = \left(33.34R - 46.31\right)\varepsilon_m + 472.31$$

Maxwell Garnett Theory
Non-Dilute Colloidal Solutions

Ref: J. C. Maxwell Garnett, Philos. Trans. R. Soc. London, 203 (1904) 385.



(a) Silica Coated Gold Particle; (b) Ideal Packing of Silica Coated Gold Particles in the Film to Form FCC Lattice with Volume Fraction 0.74.

Average Electric Field in Composite Material

$$E_{av} = (1-\phi)E_m + \phi E_p$$

E_p – Electrical Field in the Particle

E_m – Electrical Field in the Matrix Material

Particle Volume Fraction

$$\phi = \frac{0.74 R_{Au}^3}{\left(R_{Au} + R_{SiO_2}\right)^3}$$

R_{Au} – Radius of the Gold Core

R_{SiO2} – Thickness of SiO_2 Shell

Average Polarization in Composite Material

$$P_{av} = (1-\phi)(\varepsilon_m - 1)\varepsilon_0 E_m + \phi(\varepsilon_p - 1)\varepsilon_0 E_p = (\varepsilon_{av} - 1)\varepsilon_0 E_{av}$$

Electric Field Inside the Particles (Lorentz Cavity Field)

$$E_p = \frac{3\varepsilon_m}{\varepsilon_p + 2\varepsilon_m} E_m$$

ε_m – Dielectric Function of the Matrix Material

Final Form of the Equations

Average Electric Field in Composite Material

$$E_{av} = (1-\phi)E_m + \frac{3\phi\varepsilon_m}{\varepsilon_p + 2\varepsilon_m} E_m$$

Average Dielectric Function in Composite Material

$$\varepsilon_{av} = \varepsilon_m \frac{\varepsilon_p(1+2\phi) + 2\varepsilon_m(1-\phi)}{\varepsilon_p(1-\phi) + \varepsilon_m(2+\phi)}$$

Average Absorption Coefficient in Composite Material

$$\alpha_{av} = \frac{\omega}{c}\frac{\mathrm{Im}(\varepsilon_{av})}{n_{av}} = \frac{4\pi k_{av}}{\lambda}$$

Complex Dielectric Function

$$\varepsilon_i = \varepsilon_i' + i\varepsilon_i'' = (n_i + ik_i)^2 \qquad (i = ddl, av)$$

Complex Refractory Index

$$n_i = \left(\frac{\sqrt{\varepsilon_i'^2 + \varepsilon_i''^2} + \varepsilon_i'}{2} \right)^{1/2} \qquad (i = ddl, av)$$

$$k_i = \left(\frac{\sqrt{\varepsilon_i'^2 + \varepsilon_i''^2} - \varepsilon_i'}{2} \right)^{1/2} \qquad (i = ddl.av)$$

Optical Reflectance

$$R = \frac{(n_i - 1)^2 + k_i^2}{(n_i + 1)^2 + k_i^2} \qquad (i = ddl, av)$$

Optical Transmittance

$$T = \frac{(1 - R)^2 + 4R\sin^2\psi}{R^2\exp(-\alpha_i h) + \exp(\alpha_i h) - 2R\cos(\xi + 2\psi)} \qquad (i = ddl, av)$$

h – Thickness of the Au@SiO_2 Film

Optical Reflectance

$$R = \frac{(n_i - 1)^2 + k_i^2}{(n_i + 1)^2 + k_i^2} \qquad (i = ddl, av)$$

Optical Transmittance

$$T = \frac{(1 - R)^2 + 4R\sin^2\psi}{R^2\exp(-\alpha_i h) + \exp(\alpha_i h) - 2R\cos(\xi + 2\psi)} \qquad (i = ddl, av)$$

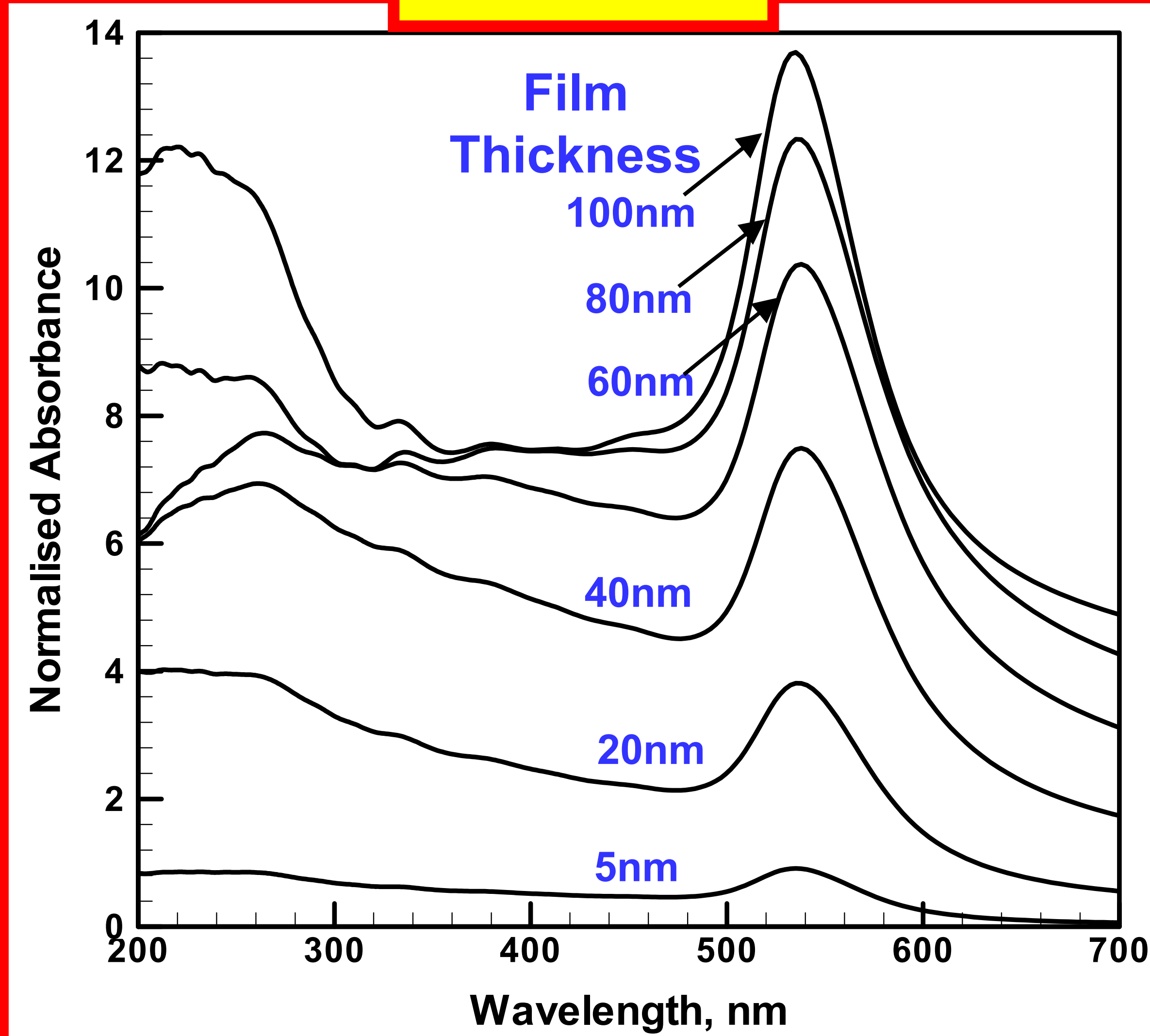
h – **Thickness of the Au@SiO_2 Film**

Functions in the Above Equation

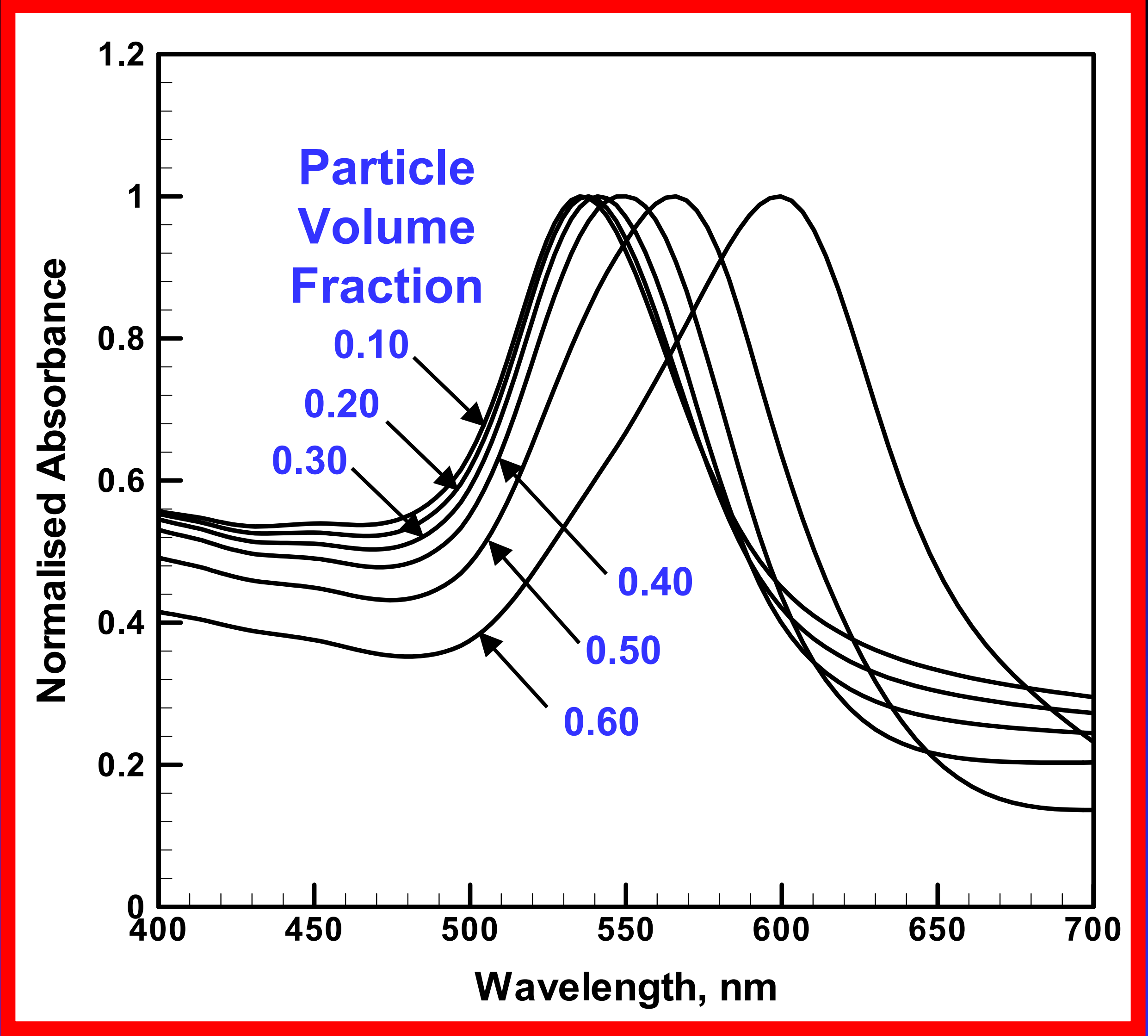
$$\xi = \frac{4\pi n_i h}{\lambda} \qquad (i = ddl, av)$$

$$\psi = \tan^{-1}\left(\frac{2k_i}{n_i^2 + k_i^2 - 1}\right) \qquad 0 \le \psi \le \pi \qquad (i = ddl, av)$$

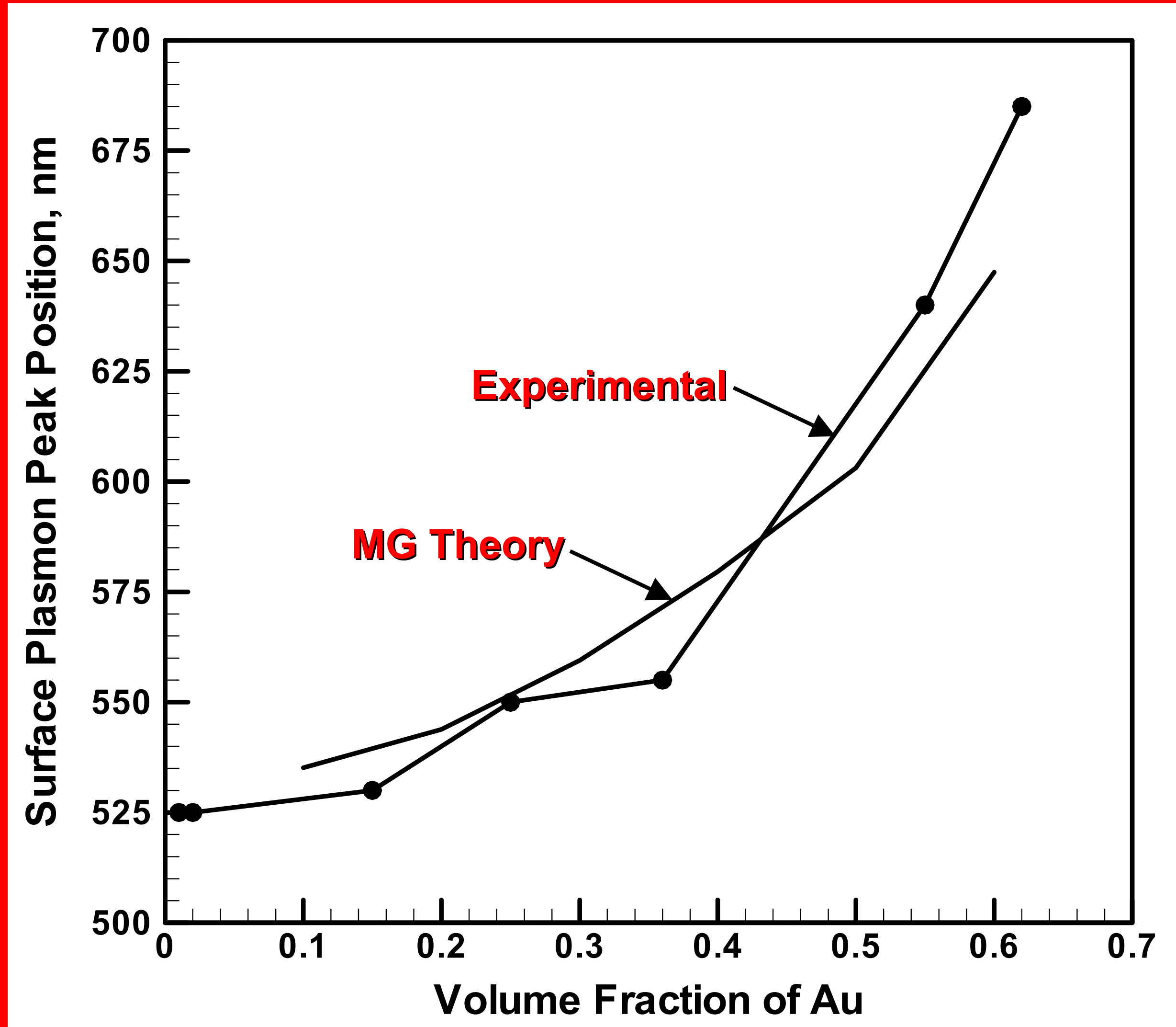
Results



Effect of Film Thickness on the Calculated Absorption Spectra of Au@SiO_2 Films at the Particle Volume Fraction ϕ = 0.05.

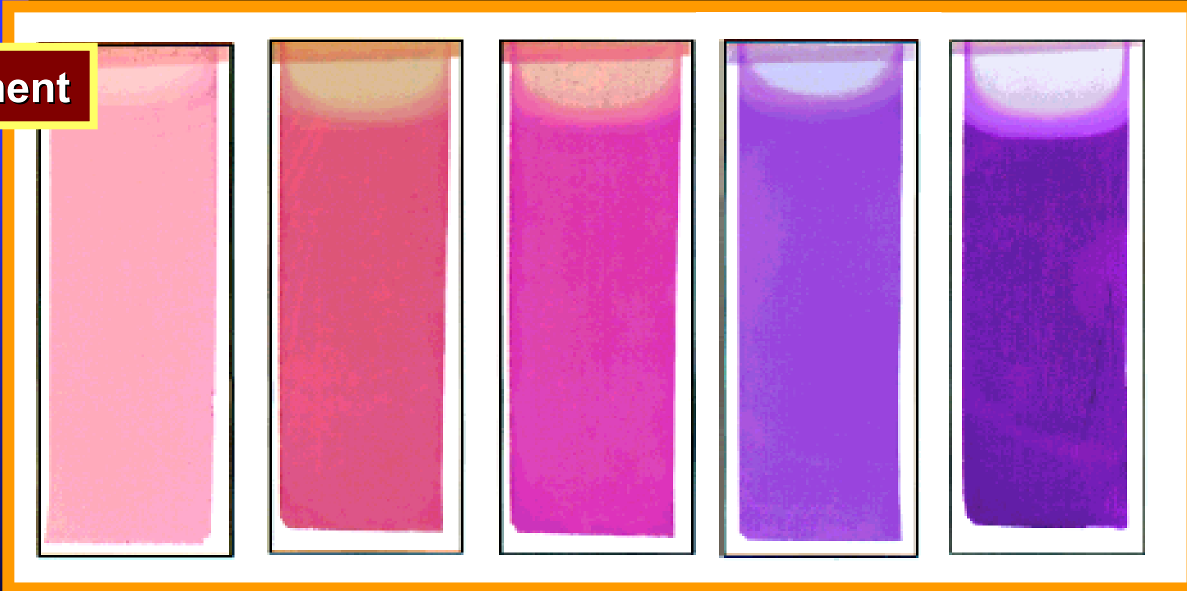


Calculated Absorption Spectra of Au Particles With Different Particle Volume Fractions.



Effect of the Particle Volume Fraction on the Calculated Peak Positions of the Coupled Plasmon Bands in Au@SiO_2 Films

Experiment

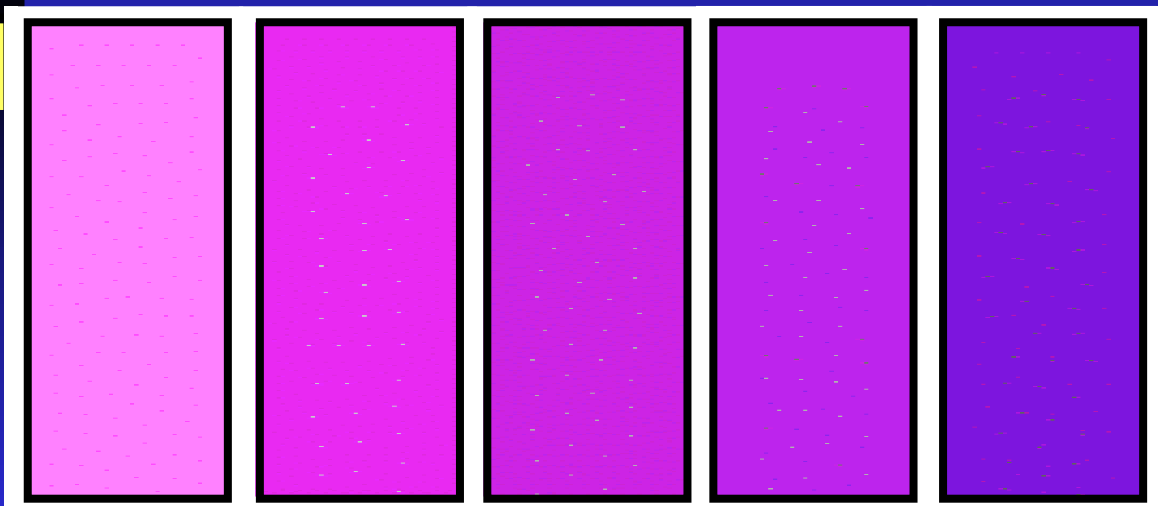


15 nm Gold Spherical Particles Coated with Silica Shells of Various Thickness

Ref: T. Ung, L. M. Liz-Marzan and P. Mulvaney, J. Phys. Chem., B105 (2001) 3441-3452

t=17.5nm	t=12.5nm	t=4.6nm	t=2.9nm	t=1.5nm

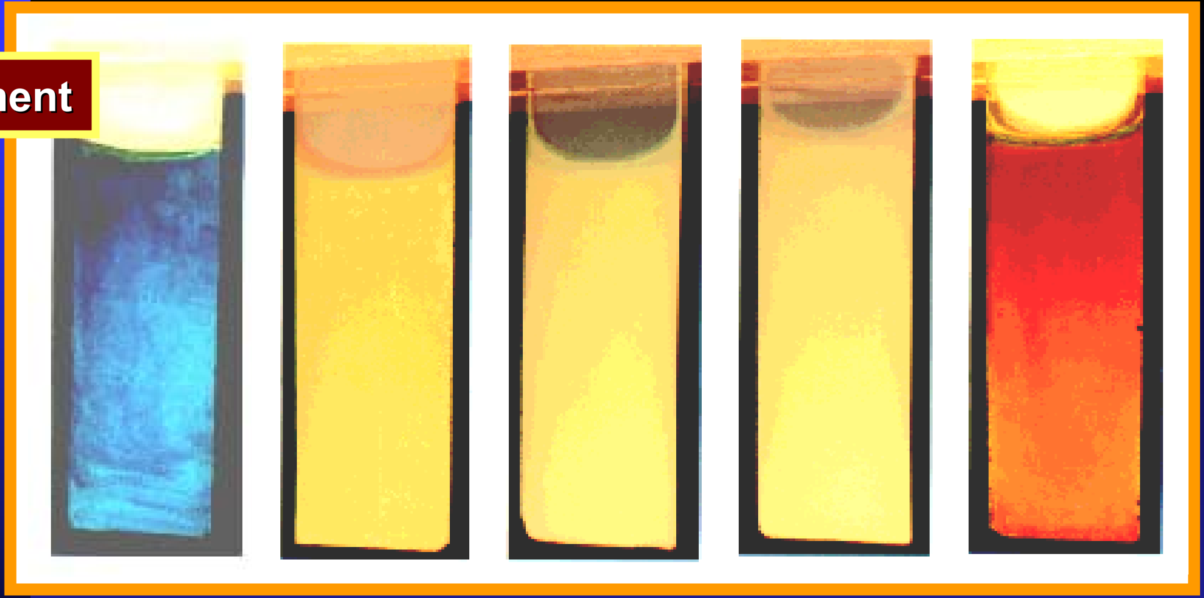
Theory



Maxwell-Garnett Theory Transmission Colors

Spherical Gold Particles
Effect of Dielectric Constant of the Medium

Experiment



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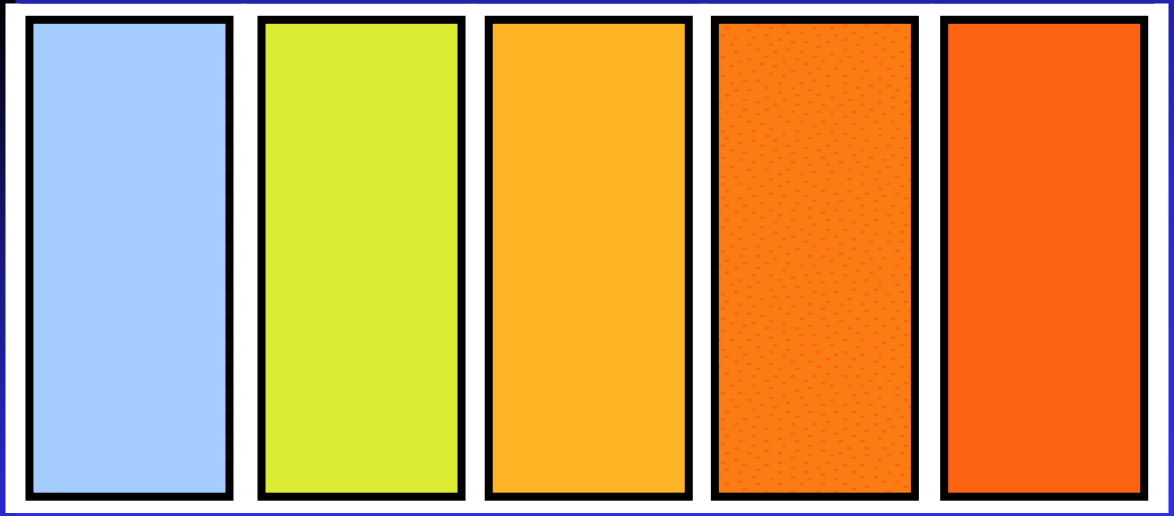
t=17.5nm	t=12.5nm	t=4.6nm	t=2.9nm	t=1.5nm

Theory



Maxwell-Garnett Theory Reflection Colors

Spherical Gold Particles
Effect of Dielectric Constant of the Medium

Discrete Dipole Approximation

Ref: J. J. Goodman, B. T. Draine, and P. J. Flateau, Opt. Lett. 16 (1991) 1198.

Polarization of Each Dipole

$$\mathbf{P}_i = \boldsymbol{\alpha}_i \cdot \mathbf{E}_i$$

α_i – Polarizability of the Dipole at r_i

Total Electricl Field at Position r_i

$$\mathbf{E}_i = \mathbf{E}_{inc,i} + \mathbf{E}_{self,i}$$

Electric Field of Incident Plain Wave

$$\mathbf{E}_{inc,i} = \mathbf{E}_0 \exp\left(i\mathbf{k}\cdot\mathbf{r}_i - i\omega t\right)$$

E_0 – The Amplitude of the Incident Electric Field

k – Wave Vector

t – Time

ω – Frequency

Electric Field From Other Dipoles

$$\mathbf{E}_{self,i} = -\sum_{j\neq i}^{N} \mathbf{A}_{ij}\cdot\mathbf{P}_j$$

Final Equation for Polarization

$$(\boldsymbol{\alpha}_i)^{-1}\mathbf{P}_i + \sum_{j\neq i}^{N}\mathbf{A}_{ij}\cdot\mathbf{P}_j = \mathbf{E}_{inc,i}$$

Dyadic Green's Function Approach

$$\mathbf{A}_{ij}\cdot\mathbf{P}_j = \frac{\exp(ikr_{ij})}{r_{ij}^3}\left\{k^2\mathbf{r}_{ij}\times(\mathbf{r}_{ij}\times\mathbf{P}_j)+\frac{(1-ikr_{ij})}{r_{ij}^2}\left[r_{ij}^2\mathbf{P}_j-3\mathbf{r}_{ij}(\mathbf{r}_{ij}\cdot\mathbf{P}_j)\right]\right\}$$

Matrix A'

$$\mathbf{A}'_{i-j} \equiv \begin{cases} \mathbf{A}_{ij} & i \neq j \\ 0 & i = j \end{cases}$$

Convolution

$$\mathbf{Y}_i = \sum_{j_x=0}^{2N_x} \sum_{j_y=0}^{2N_y} \sum_{j_z=0}^{2N_z} \mathbf{A}'_{i-j} \cdot \mathbf{P}_j \equiv \sum_j \mathbf{A}'_{i-j} \cdot \mathbf{P}_j$$

Discrete Fourier Transform

$$\hat{\mathbf{Y}}_n \equiv \sum_i \mathbf{Y}_i \exp\left[i \left(\frac{n_x i_x}{2N_x} + \frac{n_y i_y}{2N_y} + \frac{n_z i_z}{2N_z} \right) \right]$$

Extinction Cross Section

$$C_{ext} = \frac{4\pi k}{|\mathbf{E_0}|^2} \sum_{i=1}^{N} \mathrm{Im}\left(\mathbf{E}_i^* \cdot \mathbf{P}_i\right)$$

E_i^* – Complex Conjugate of Total Electric Field at r_i

Absorption Cross Section

$$C_{abs} = \frac{4\pi k}{|E_0|^2} \sum_{i=1}^{N} \left\{ \mathrm{Im}\left[\mathbf{P}_i \cdot \left(\alpha_i^{-1}\right)^* \mathbf{P}_i^*\right] - \frac{2}{3} k^3 |\mathbf{P}_i|^2 \right\}$$

Scattering Cross Section

$$C_{sca} = C_{ext} - C_{abs}$$

Reflectivity

$$R = \frac{\left[\cos(\theta_i) - m\cos(\theta_r)\right]^2}{\left[\cos(\theta_i) + m\cos(\theta_r)\right]^2}$$

θ_i - Incident Angle

θ_r -Refractive Angle

Complex Refractory Index

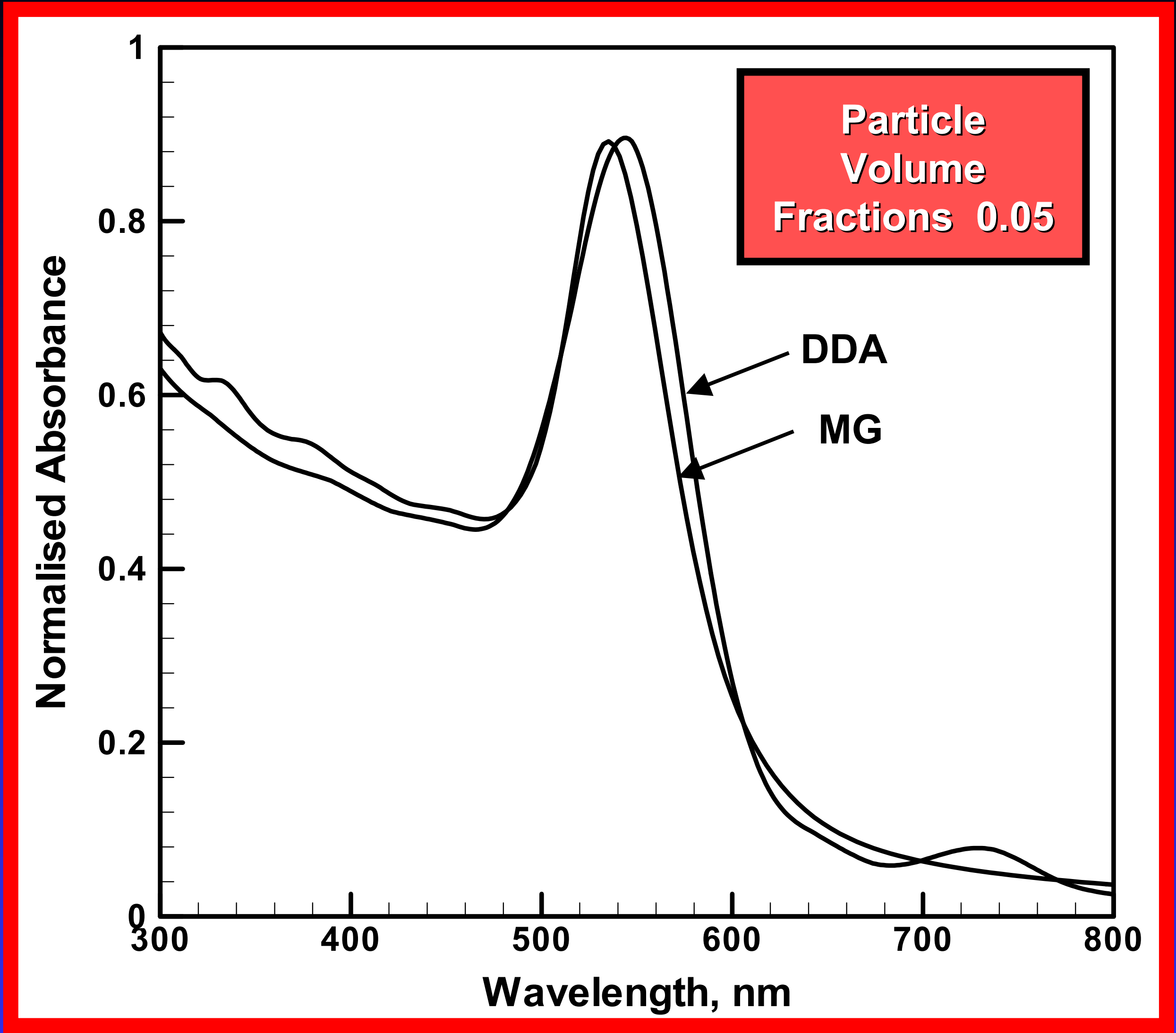
$$m = n + ik$$

Imaginary Part of Refractory Index

$$k = \left(m^2 - n^2\right)^{1/2}$$

Real Part of Refractory Index

$$n = \sin\left(\theta_i\right) / \sin\left(\theta_r\right)$$

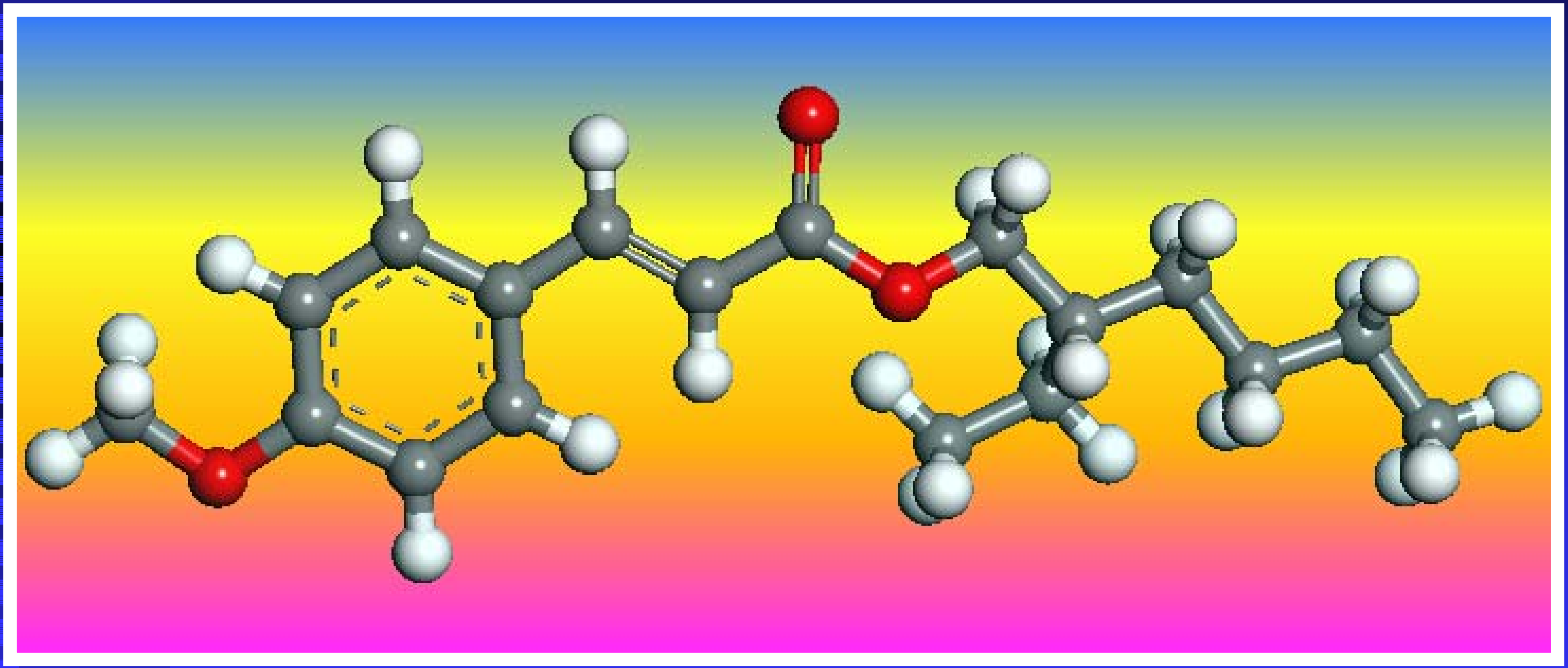


Comparison of the Calculated Results from DDA and MG Effective Medium Method

UV Spectra of Molecules

Ref: Accelrys VAMP Tutorial

Cinnamate Molecule



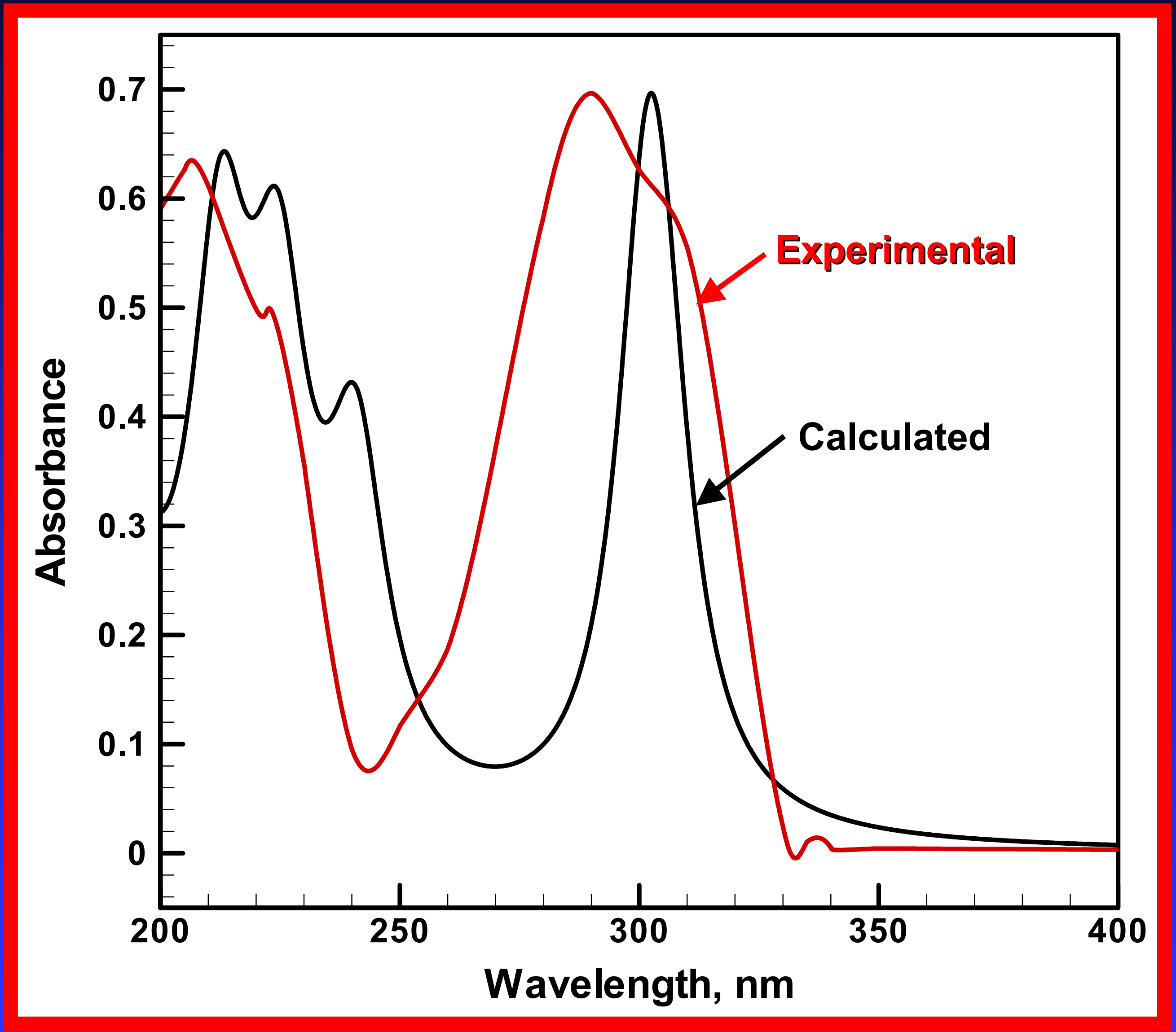
- Although self-consistent field calculations are adequate for the vast majority of ‘normal’ molecules, biradicals and excited states require a more sophisticated treatment.
- This is often achieved using configuration interaction methods (CI). In CI calculations, the molecular orbitals for the ground state are calculated and then used unchanged to construct a series of further electronic configurations (microstates) that are mixed to form new electronic states.
- CI calculations give not only the ground state, but also the excited states that result from mixing the microstates used. They can therefore be used for the calculation of UV/vis spectra, optimization of excited states, second order hyperpolarizabilities (sum-over-states method) etc.
- CI calculations are available only for RHF wavefunctions. Any spin state (single, doublet, etc.) can be requested.

Configuration Interaction Results

Ground State	Excited State	Energies		Del Mu	Dipole Length, A			|r|	Osc. Str.
		ev	nm		|x|	|y|	|z|		
1	5	4.060	305.3	0.38	-0.210	0.388	-0.018	0.441	0.069
1	6	4.111	301.6	2.85	0.282	-1.007	0.048	1.047	0.394
1	9	5.147	240.9	5.31	0.247	-0.581	0.031	0.632	0.180
1	10	5.518	224.7	3.60	0.776	0.274	0.010	0.824	0.327
1	11	5.834	212.5	0.89	-0.101	0.944	-0.025	0.950	0.461
1	15	6.518	190.2	4.77	-0.329	0.106	0.050	0.349	0.070
1	16	6.653	186.3	6.53	0.520	0.206	-0.020	0.560	0.182
1	19	7.128	173.9	1.72	-0.005	0.191	-0.019	0.192	0.023
1	20	7.339	168.9	3.55	-0.142	-0.116	0.000	0.183	0.022

Accelrys' VAMP

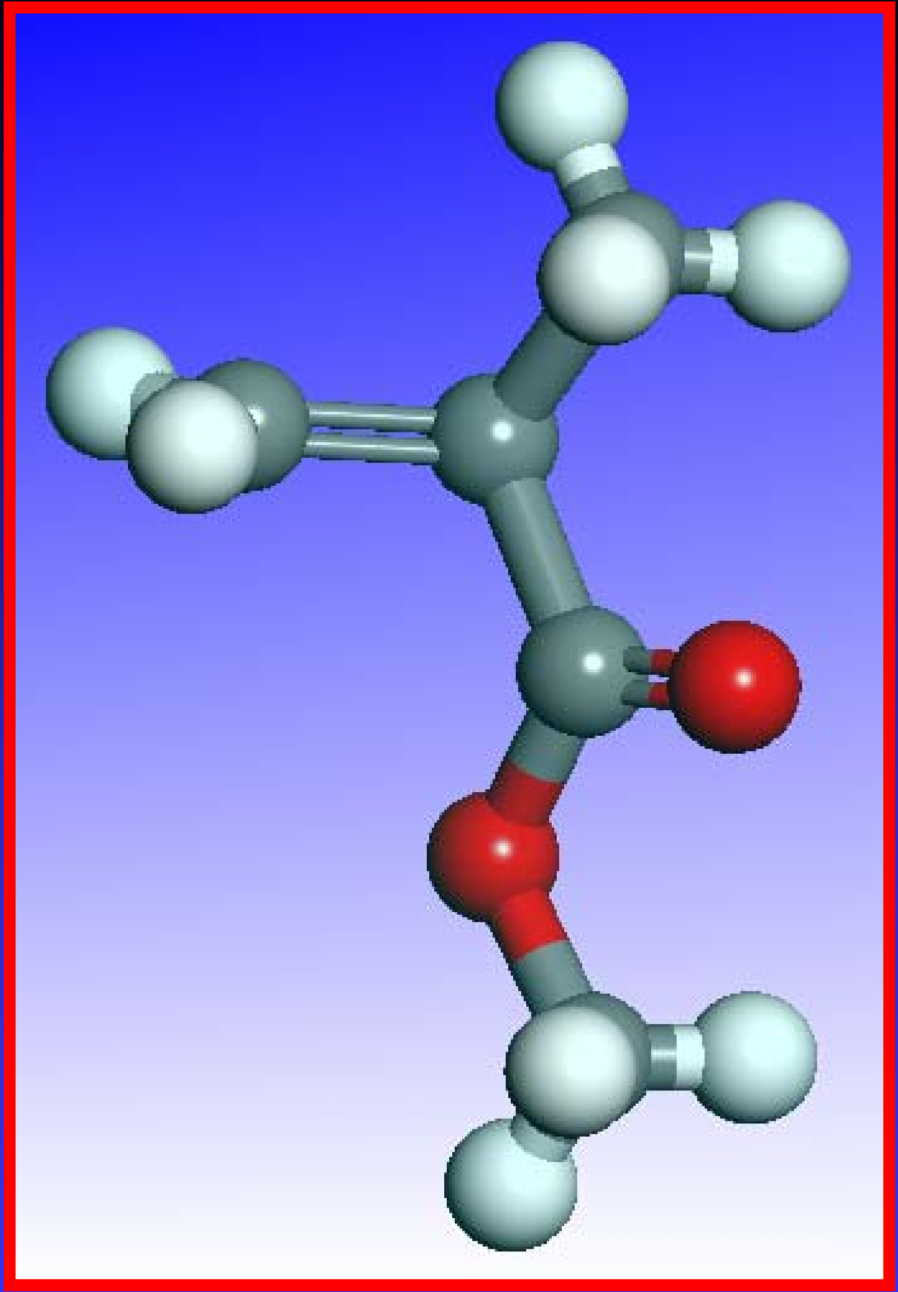
Adsorption Spectrum for Cinnamate



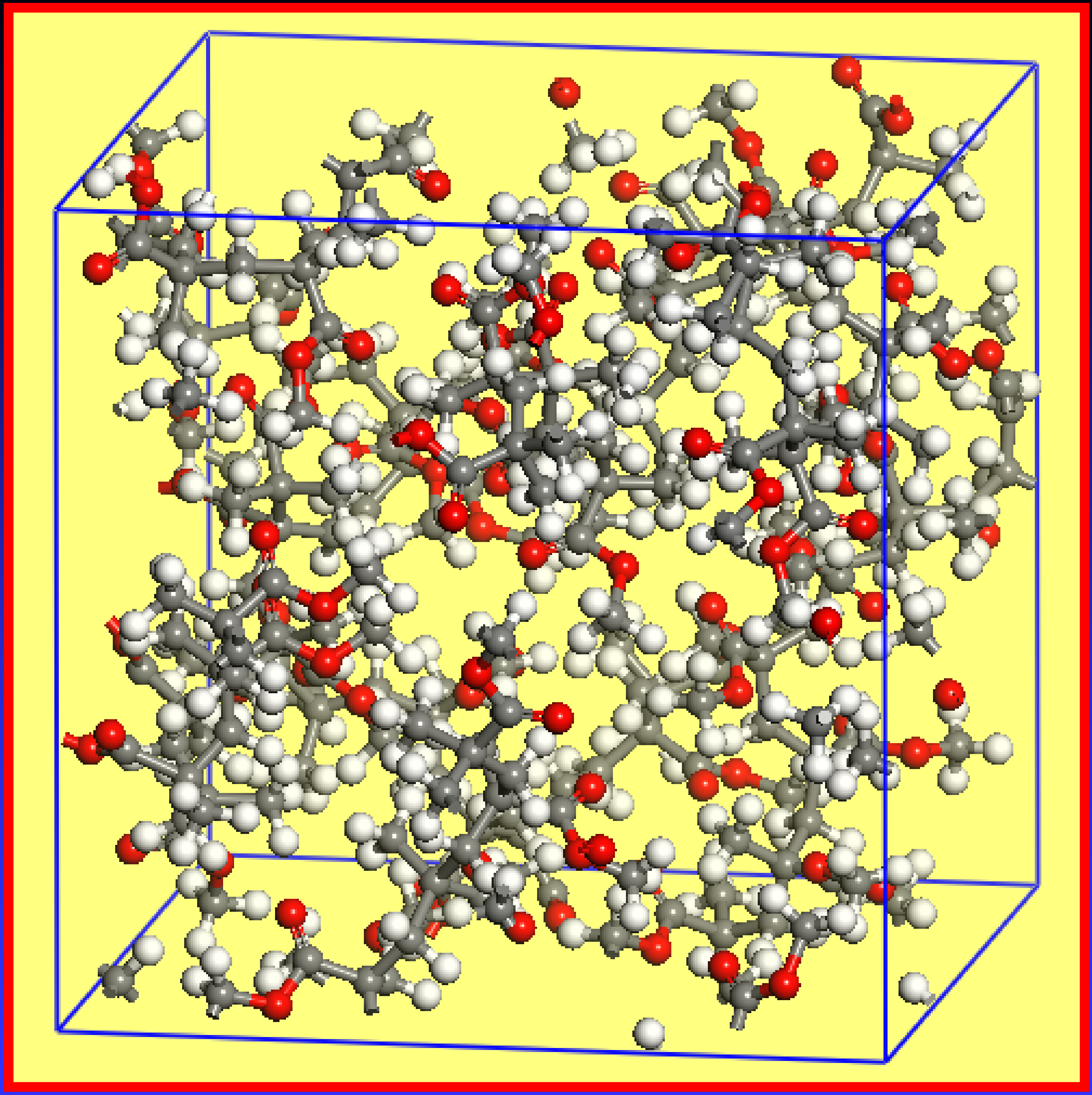
IR Spectra of Polymers

Ref: A. Soldera and J.-P. Dognon, “Optical Coefficients of Polymers Versus Wavelength Calculated From Classical Molecular Simulations”, ACS Division of Polymeric Materials, Science and Engineering, 75 (1996) 227-228.

Methyl-Metha-Acrylate (MMA)



Poly-Methyl-Metha-Acrylate (PMMA)



Normal Mode Analysis

Accelrys' Discover

Mode	Frequency 1/cm	Intensity km/mol
0	0.0000	0.0000
1	0.0000	0.0000
2	0.0002	0.0000
3	10.5047	0.4503
4	11.0933	0.1346
5	12.0889	0.1937
6	13.7781	0.0251
7	14.0765	0.2983
8	15.6383	0.2285
9	15.9993	0.1383
10	17.2644	0.0848
11	18.1106	0.3391
12	18.6154	0.1507

Infra Red Absorption Coefficient (Ramsay Function)

$$K(\nu) = \frac{1}{V_m} \sum_i \left[\frac{2S_i}{2.303\pi} \Delta\nu_{1/2} \frac{1}{4(\nu - \nu_i)^2 + \Delta\nu_{1/2}^2} \right]$$

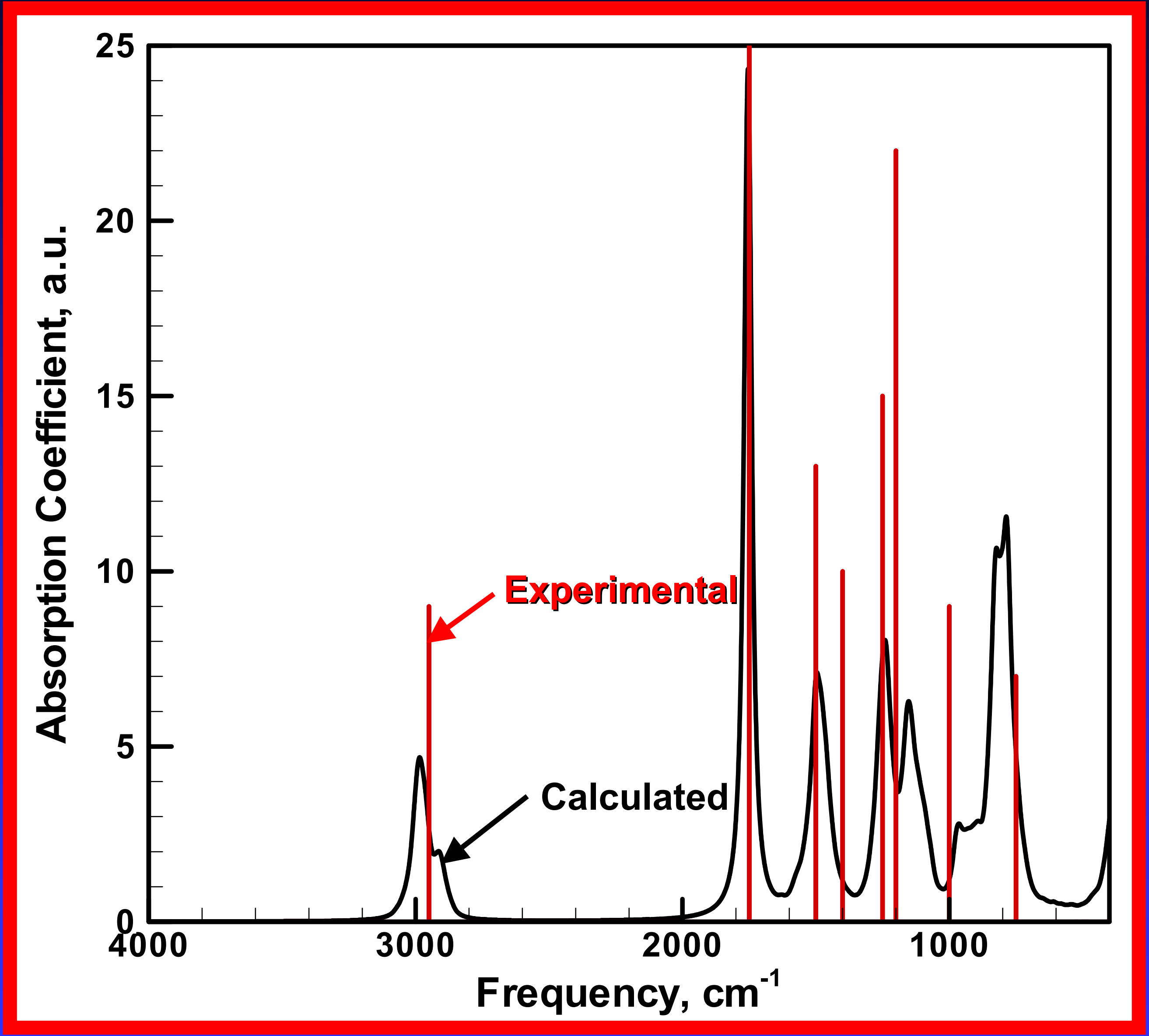
ν_i - Wavenumber

$\nu_{1/2}$ - Half Width

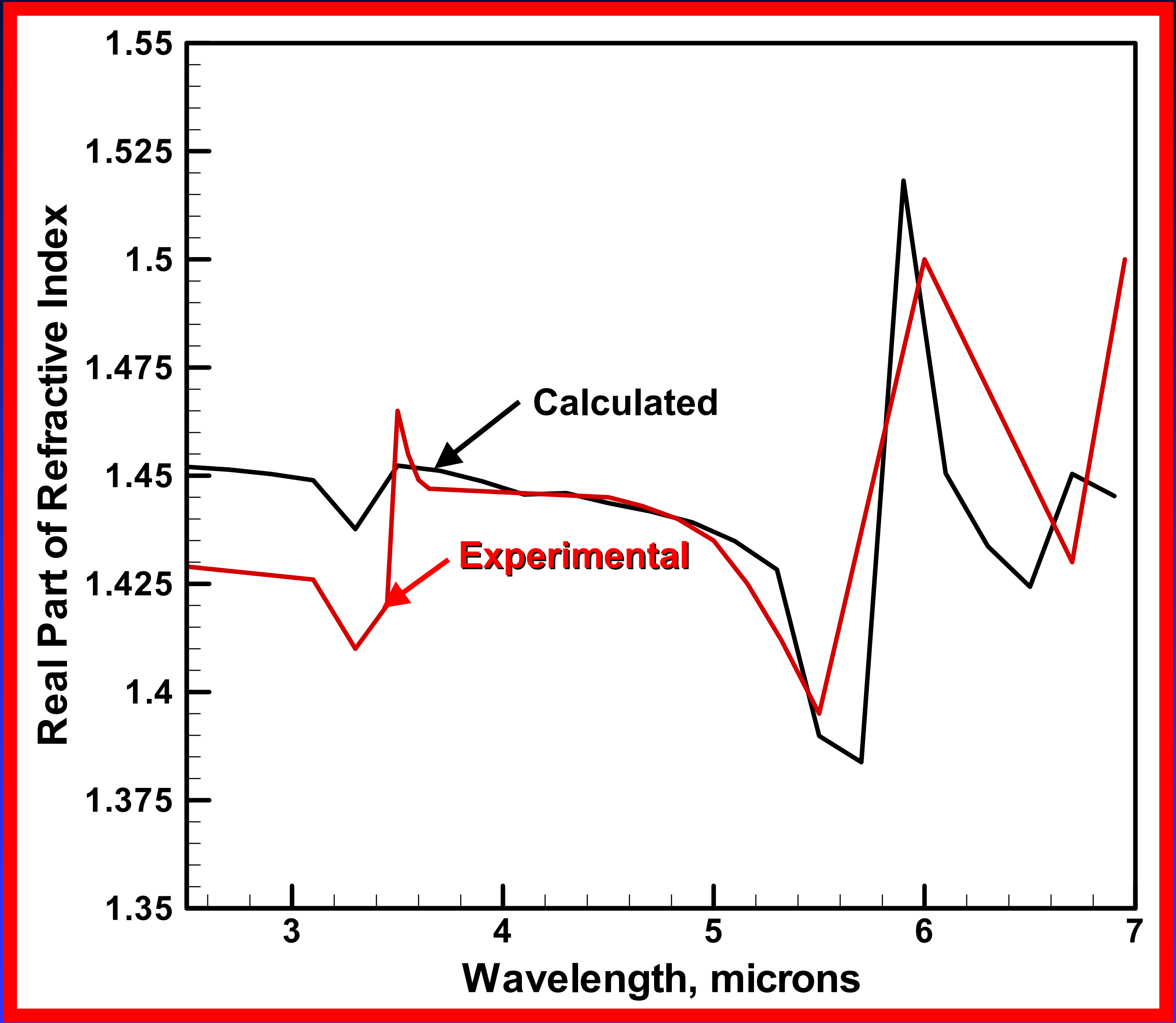
V_m - Molar Volume

S_i - Integrated Intensity

Infrared Absorption Spectra of PMMA



Real Part of Refractive Index of PMMA



Polymer Colloidal Crystal Photonic Bandgap Structure

S.H. Foulger, D.W. Smith, Jr. and J. Ballato
Clemson University

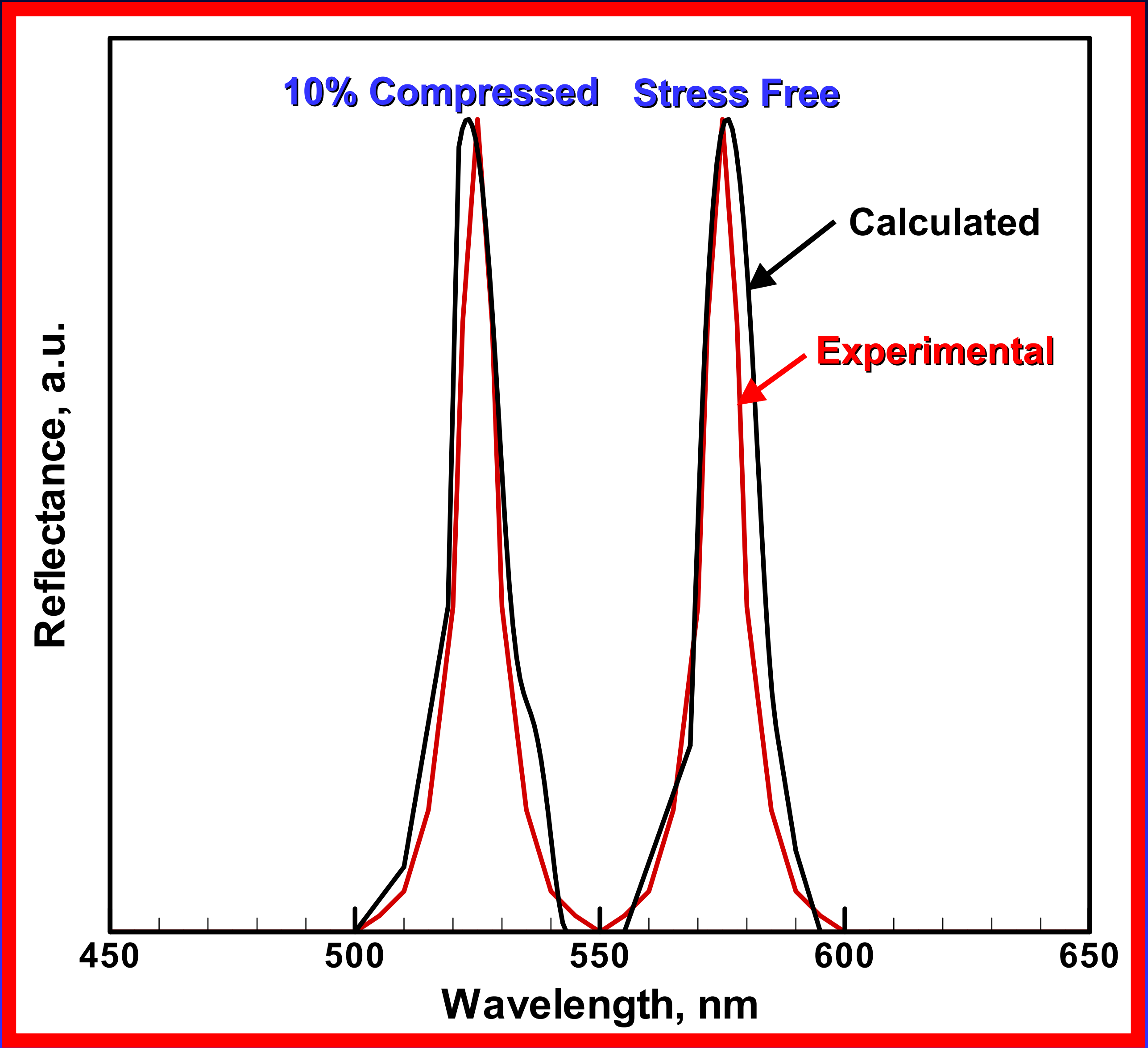
A.L. Reynolds – "Translight": A Transfer Matrix Code
http://www.elec.gla.ac.uk/groups/opto/photoniccrystal/Photonics/photonicsmain.htm

Structural and Optical Parameters of Polymer Encapsulated FCC Crystalline Colloidal Arrays

Type	Particles	Particle Diameter (nm)	Particle Distance (nm)	Capping Medium
CCA	Polystyrene	93	185.2	Water, n = 1.344
CCA/PEG	Polystyrene	93	198.9	Water + Poly(ethylene glycol) methacrylate (PEG-MA) + Poly(ethylene glycol) dimethacrylate (PEG-DMA) 2,2-diethoxyacetophenone(DENP) n = 1.367
PCCA	Polystyrene	93	198.3	Polymerized State of the Above n = 1.368

Ref: S. H. Foulger, et. al., Langmuir, 17 (2001) 6023

Mechanochromic Response of PCCA Composite

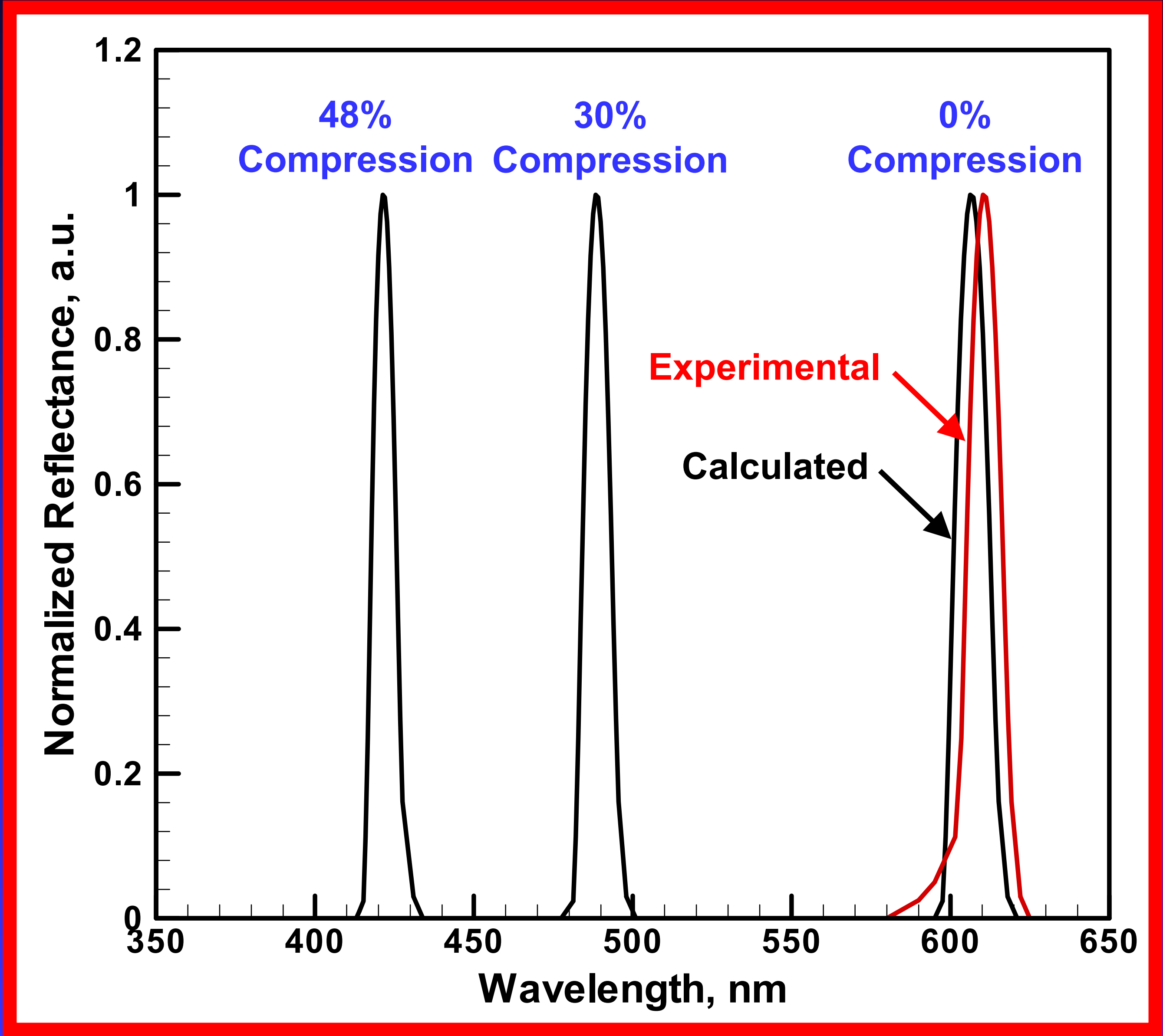


Structural and Optical Parameters of Polymer Encapsulated FCC Crystalline Colloidal Arrays

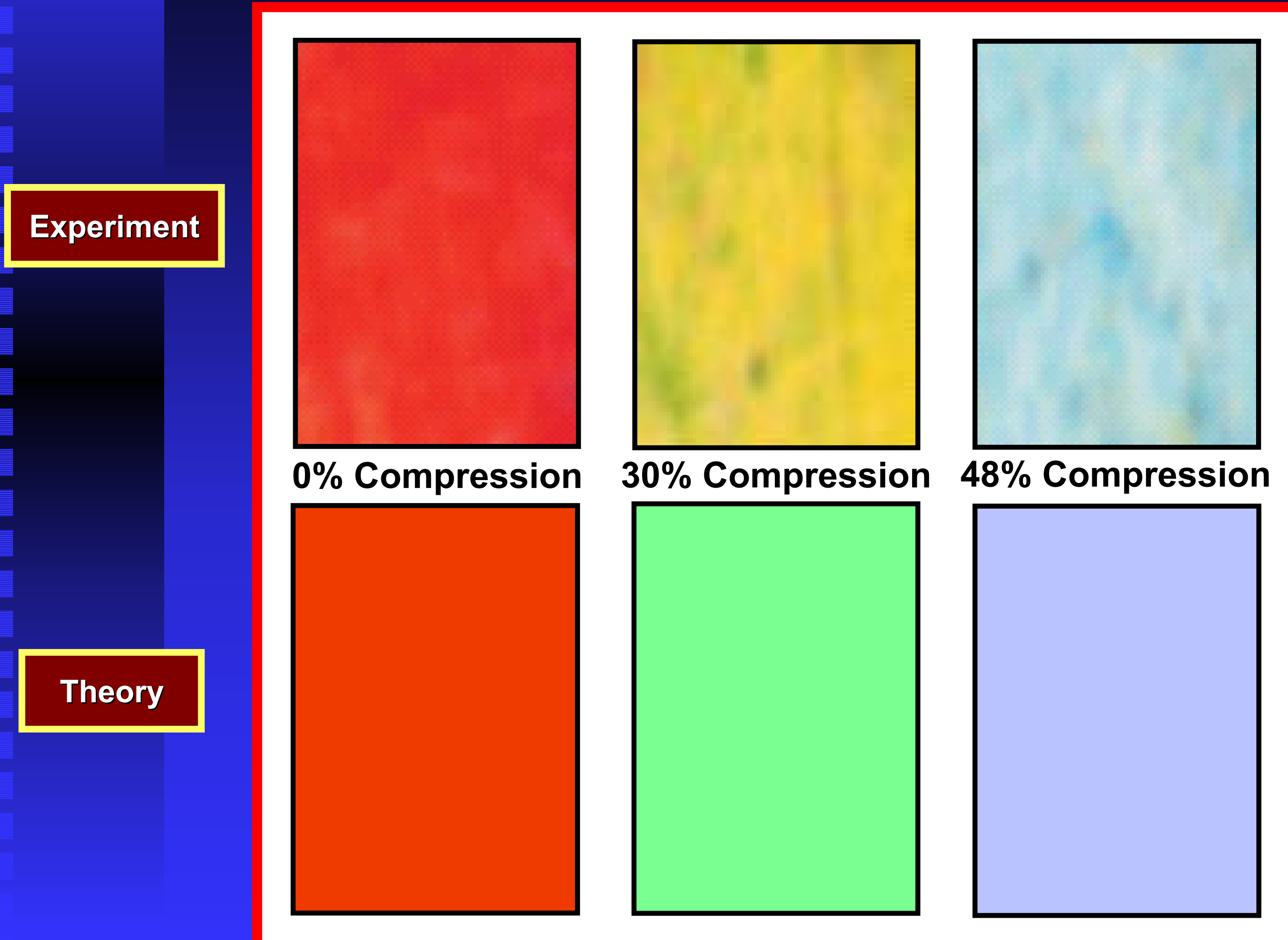
Type	Particles	Particle Diameter (nm)	Particle Distance (nm)	Capping Medium
MOEA	Polystyrene	109	203	Poly(ethylene glycol) + Poly(2-methoxyethyl acrylate (MOEA)) ,(n_c = 1.489)
MOEA+ MOEM (50:50)	Polystyrene	109	203	Poly(ethylene glycol) + Poly(2-methoxyethyl acrylate)-co-poly(2-methoxyethyl methacrylate)
MOEM	Polystyrene	109	203	Poly(ethylene glycol) + Poly(2-methoxyethyl methacrylate (MOEM))

Ref: S. H. Foulger, et. al., Adv. Mater., 15 (2003) 685

Calculated/Measeured Reflectance Spectra for Different Compressive Stress



A Comparison of the Measured and Calculated Reflected Colors

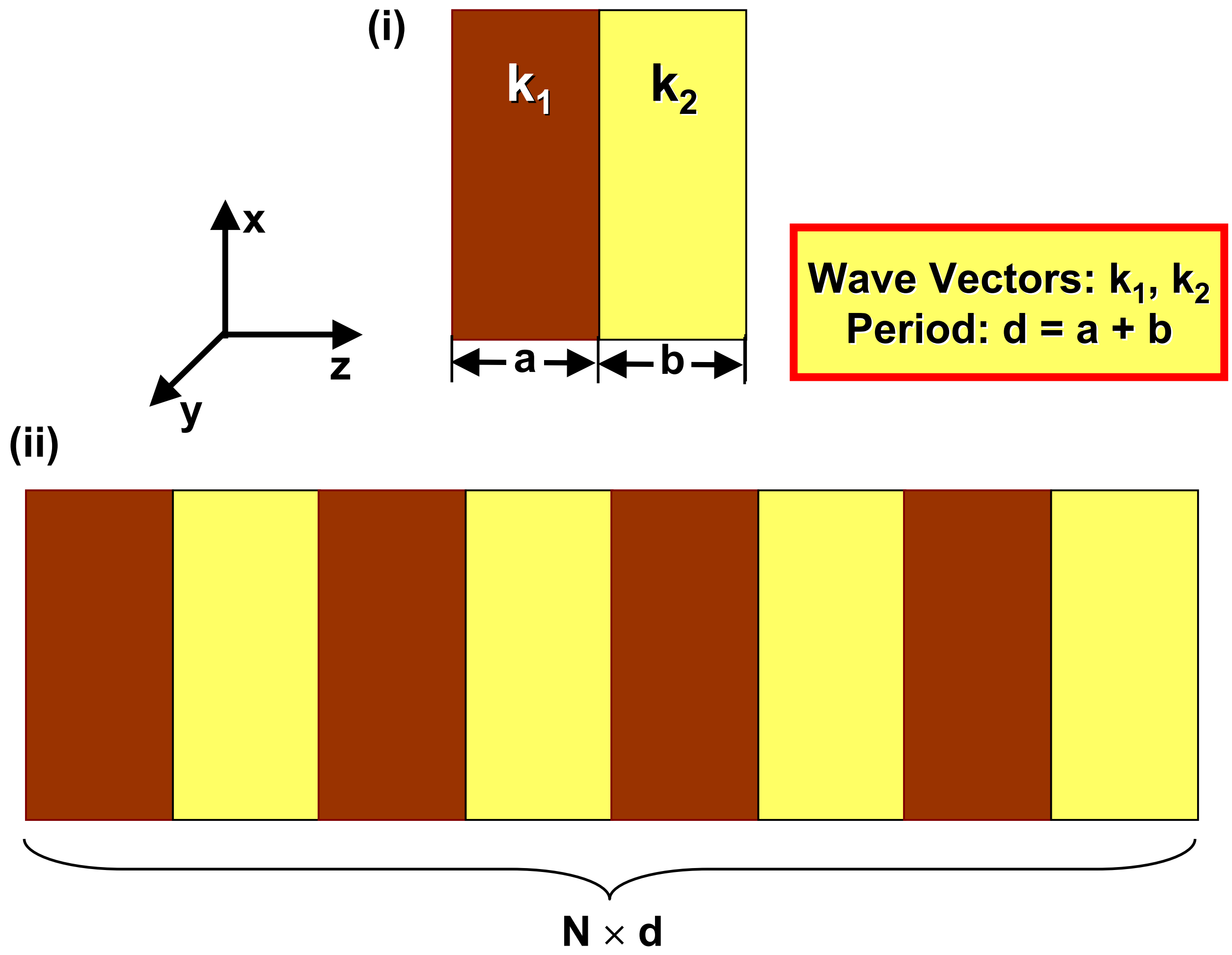


One-Dimensional Photonic Bandgap Structures

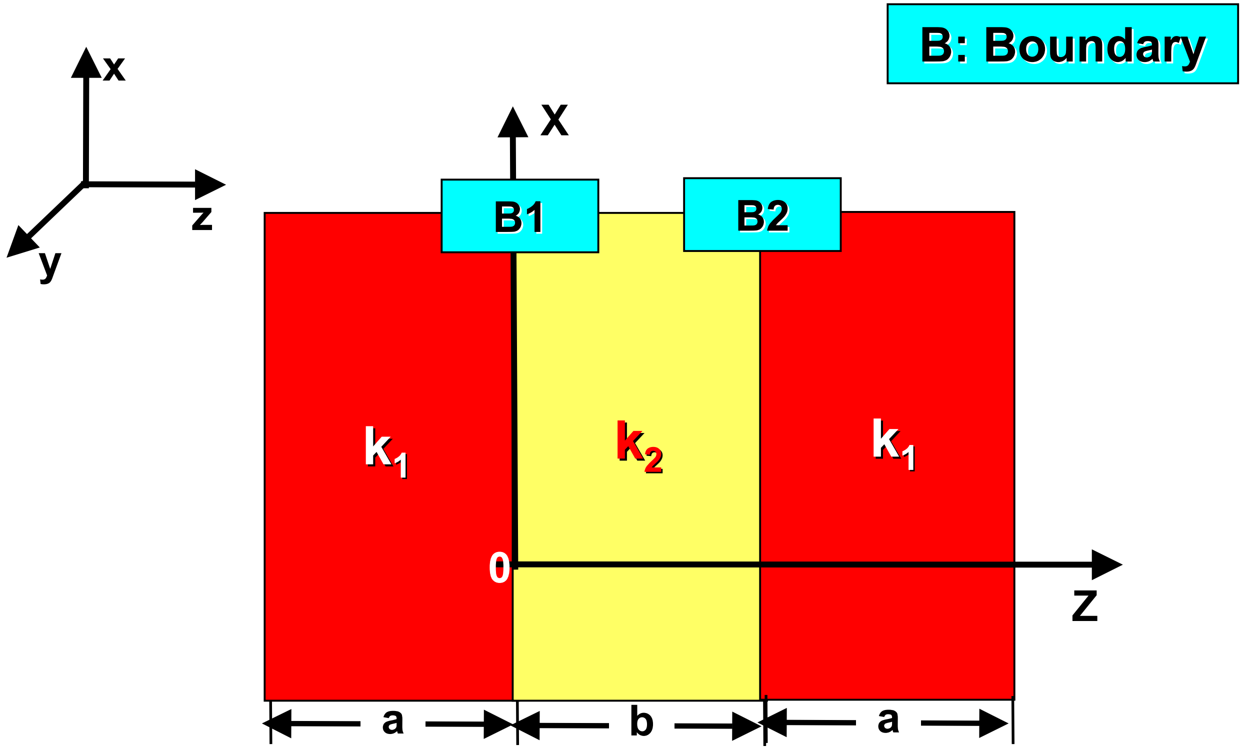
A.L. Reynolds – "Translight": A Transfer Matrix Code
http://www.elec.gla.ac.uk/groups/opto/photoniccrystal/Photonics/photonicsmain.htm

Transfer Matrix Method

One-dimension Planar Periodic Structure



(i) Two-layer Planar Structure
(ii) Periodic Two-layer Planar Structure



$$\phi = [\phi_1\ (z<0),\ \phi_2\ (0<z<b),\ \phi_3\ (z>b)]$$

Definition of the Problem

Maxwell Electromagnetic Equations

$$\nabla \times \mathbf{E} = i(\omega/c)\mathbf{H}$$

$$\nabla \times \mathbf{H} = -i(\omega/c)\varepsilon(\mathbf{r})\mathbf{E}$$

E – Electrical Field

H – Magnetic Field

ω – Angular Frequency

c – Light Speed

ε(r) – Dielectric Constant

One-Dimensional Case

$$\mathbf{E}(\mathbf{r}) = \left(E,0,0\right)$$

$$\mathbf{H}(\mathbf{r}) = \left(0,H,0\right)$$

$$\nabla \times \mathbf{E} = i\left(\omega/c\right)\mathbf{H} \quad \rightarrow \quad \frac{\partial E}{\partial z} = -\frac{i\omega}{c}H$$

$$\nabla \times \mathbf{H} = -i\left(\omega/c\right)\varepsilon\left(\mathbf{r}\right)\mathbf{E} \quad \rightarrow \quad -\frac{\partial H}{\partial z} = -\frac{i\omega}{c}\varepsilon(z)E$$

$$\frac{\partial^2 E}{\partial z^2} + \varepsilon(z)\frac{\omega^2}{c^2}E = 0$$

Boundary Conditions

At Boundary B1:

$$\phi_1 = \phi_2$$

$$\partial\phi_1/\partial z = \partial\phi_2/\partial z$$

$$\rightarrow \begin{bmatrix} C \\ D \end{bmatrix} = M_1 \begin{bmatrix} A \\ B \end{bmatrix}$$

At Boundary B2:

$$\phi_2 = \phi_3$$

$$\partial\phi_2/\partial z = \partial\phi_3/\partial z$$

$$\rightarrow \begin{bmatrix} F \\ G \end{bmatrix} = M_2 \begin{bmatrix} C \\ D \end{bmatrix}$$

Solution Form - Wave Functions

$$\phi_1 = A \cdot e^{ik_1 z} + B \cdot e^{-ik_1 z}$$

A, C, F - Incident Waves Magnitude

$$\phi_2 = C \cdot e^{ik_2 z} + D \cdot e^{-ik_2 z}$$

B, D, G - Reflected Waves Magnitude

$$\phi_3 = F \cdot e^{ik_1 z} + G \cdot e^{-ik_1 z}$$

k_1, k_2 - Wave Vector in Materials 1 and 2

$$\phi = [\mathbf{E}, \mathbf{H}]$$

E, H - Electrical, Magnetic Fields

Wave Vectors

After Substitution of ϕ_1 and ϕ_2 into the Governing Equation one Obtains:

$$k_1^2 = \varepsilon_1 \cdot (\omega^2 / c^2)$$

$$k_2^2 = \varepsilon_2 \cdot (\omega^2 / c^2)$$

Transfer Matrix

$$\begin{bmatrix} F \\ G \end{bmatrix} = T \begin{bmatrix} A \\ B \end{bmatrix}$$

$$T = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} = T_1 \cdot T_2$$

$$T_1 = \begin{bmatrix} 1 & 1 \\ k_2 & -k_2 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 \\ k_1 & -k_1 \end{bmatrix}$$

$$T_2 = \begin{bmatrix} exp(ik_1 \cdot a) & exp(-ik_1 \cdot a) \\ k_1 exp(ik_1 \cdot a) & -k_1 exp(-ik_1 \cdot a) \end{bmatrix}^{-1} \times \begin{bmatrix} exp(ik_2 \cdot a) & exp(-ik_2 \cdot a) \\ k_2 exp(ik_2 \cdot a) & -k_2 exp(-ik_2 \cdot a) \end{bmatrix}$$

Bloch Theorem

$$\phi\big|_{z=d} = \exp\left(iK\cdot d\right)\cdot \phi\big|_{z=0}$$

$$\begin{bmatrix} F \\ G \end{bmatrix} = \exp(iK\cdot d)\begin{bmatrix} A \\ B \end{bmatrix}$$

$$T(\omega)\begin{bmatrix} A \\ B \end{bmatrix} = \exp(iK\cdot d)\begin{bmatrix} A \\ B \end{bmatrix}$$

Eigevalue Problem

Band Structure Calculation

$$\det\left|T(\omega) - \exp(iK\cdot d)\cdot I\right| = 0$$

$$\cos(K\cdot d) = Func(\omega)$$

$$\omega = Func^{-1}[\cos(K\cdot d)]$$

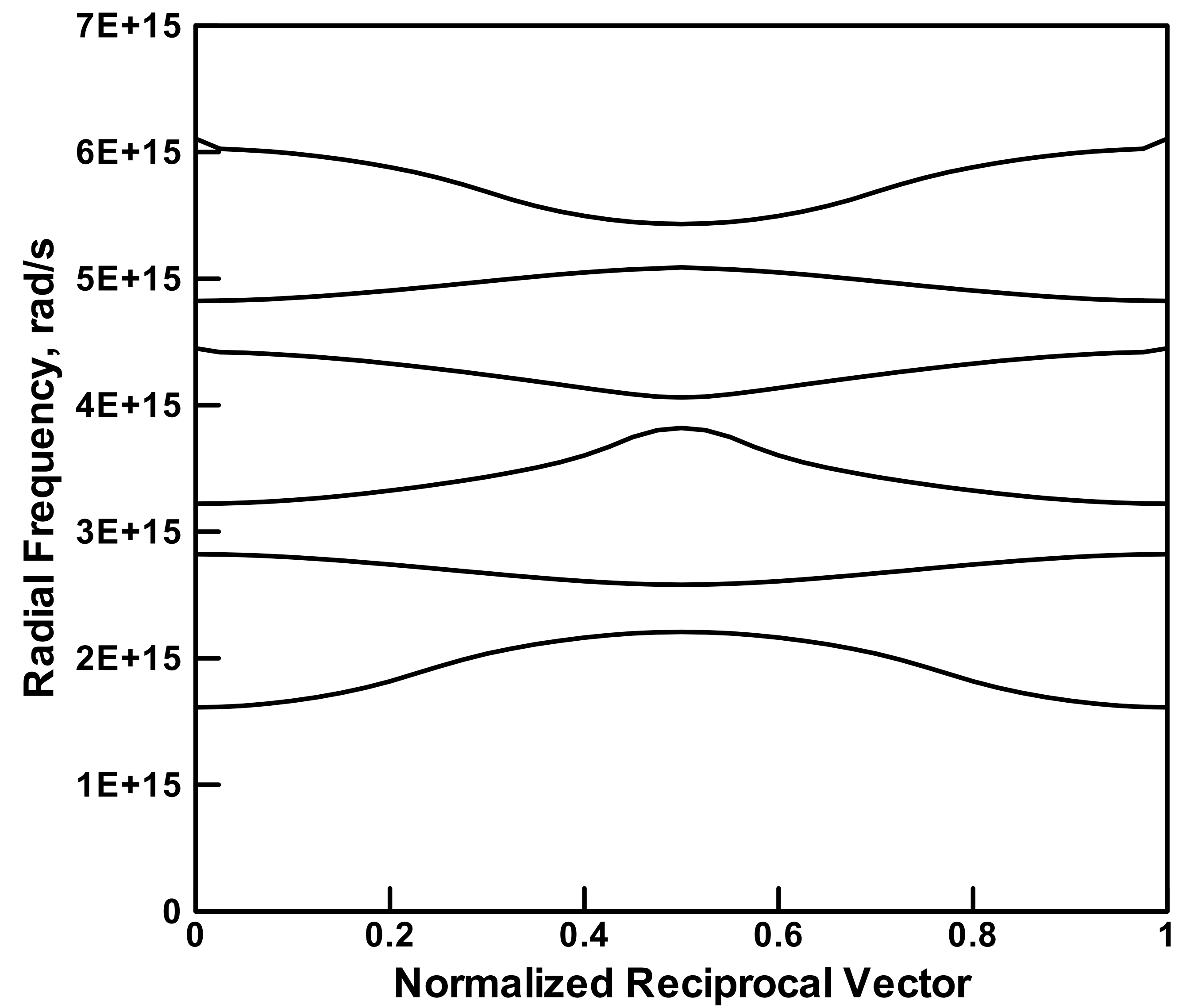
$Func^{-1}$ – A Multi-valued Function

Transmission Coefficient

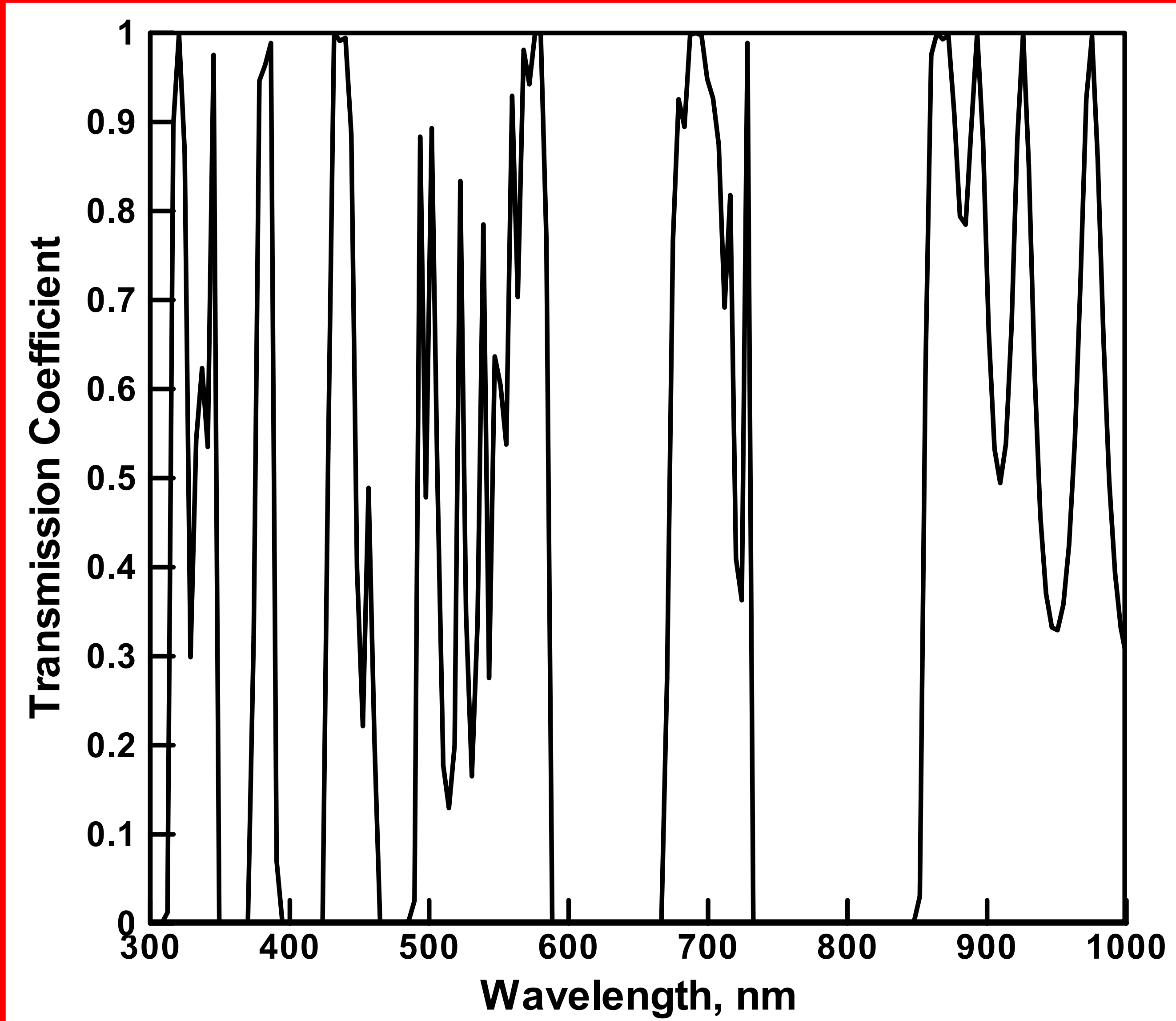
$$C_{trans} = \left| \frac{F}{A} \right|^2$$

$$C_{trans} = \left| \mathrm{Re}\, al(T_{11}^{-1}) \right|^2$$

Band Structure Calculation



Transmission Spectrum



The End