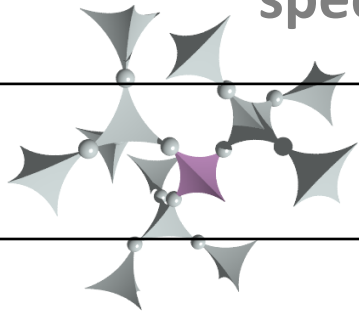


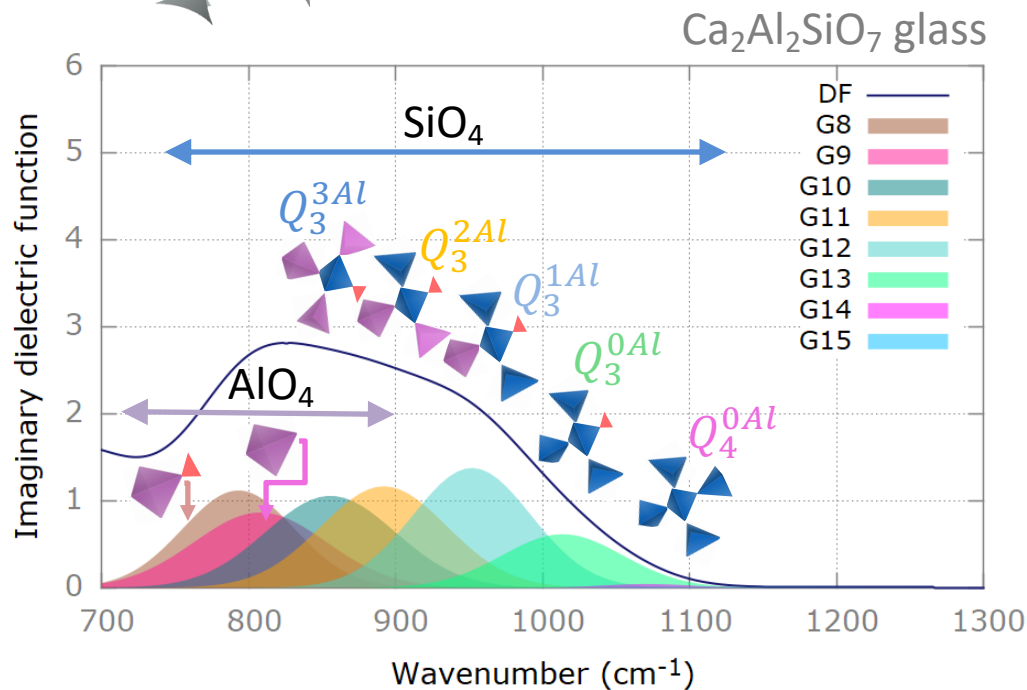
Contribution of infrared spectroscopy to the analysis of the glass structure



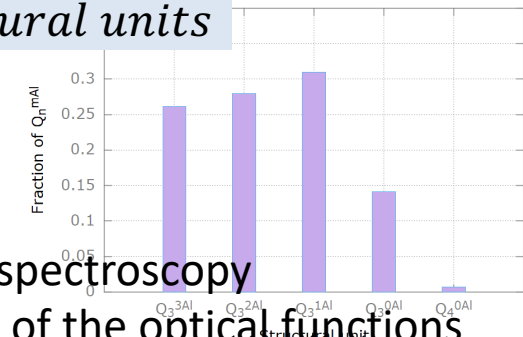
Domingos De Sousa Meneses

CEMHTI UPR3079 CNRS, Univ. Orléans, F-45071 Orléans, France

e-mail: desousa@cnrs-orleans.fr

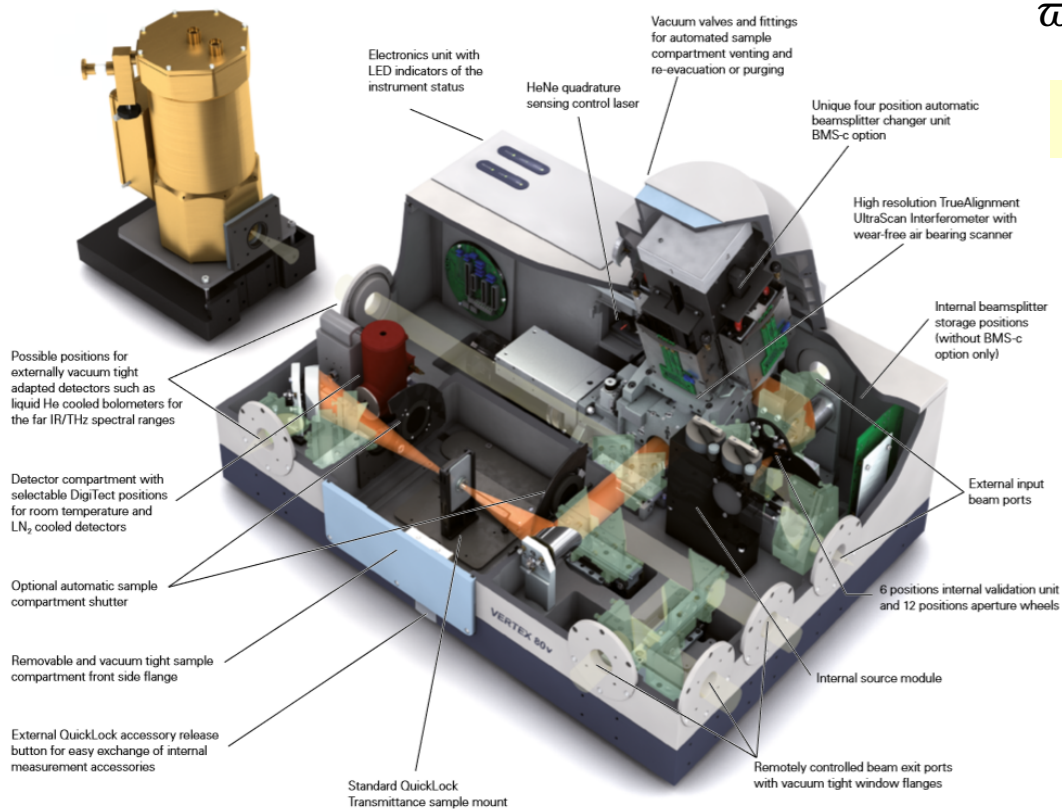
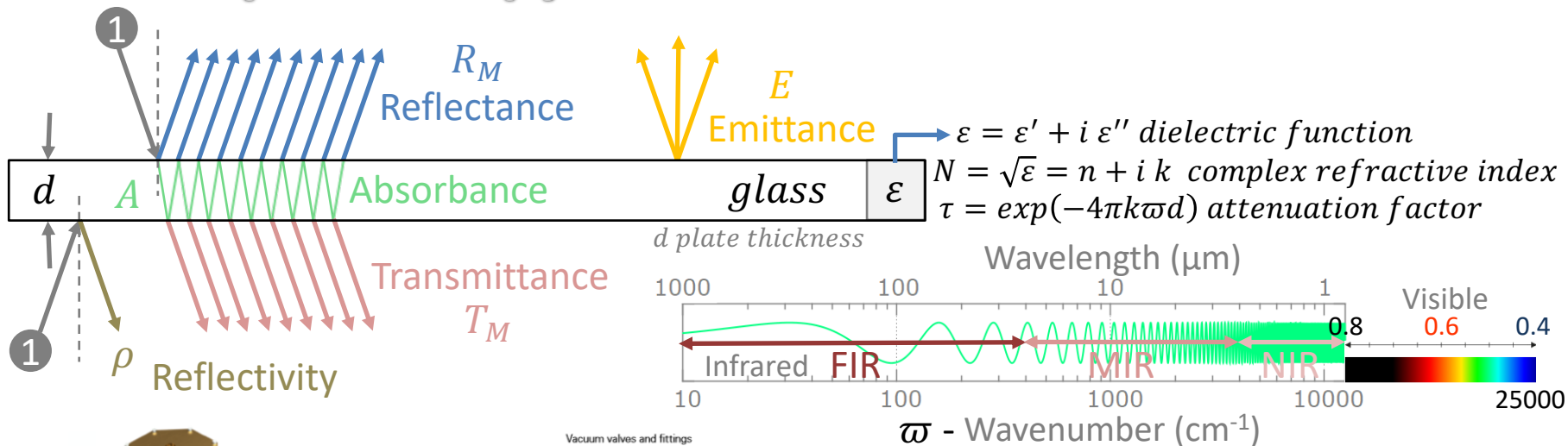


Q_n^{mAl} structural units



- ❖ Infrared spectroscopy
- ❖ Retrieval of the optical functions
- ❖ Dielectric function models
- ❖ Focus software
- ❖ Origin of the vibrational modes
- ❖ Silicates glasses
- ❖ Aluminosilicate glasses
- ❖ Iron in silicate glasses and melts

Infrared spectroscopy



Experimental observables *

Parallel plate sufficiently thick to avoid the observation of interferences

$$\text{Reflectivity } \rho = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

$$\text{Reflectance } R_M = \rho \left[1 + \frac{(1-\rho)^2 \tau^2}{1-\rho^2 \tau^2} \right]$$

$$\text{Transmittance } T_M = \tau \frac{1-\rho}{1+\rho} \frac{1-\rho^2}{1-\rho^2 \tau^2}$$

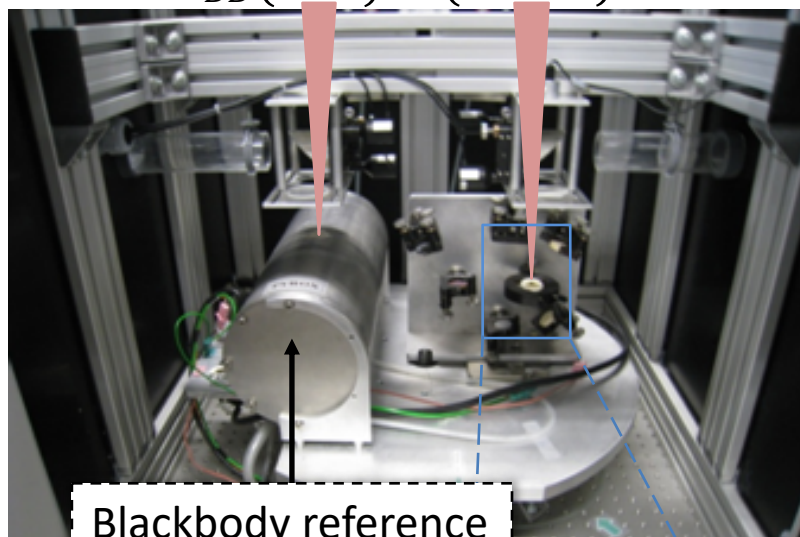
Absorbance and Emittance

$$E = A = 1 - R_M - T_M = \frac{(1-\rho)(1-\tau)}{1-\rho\tau}$$

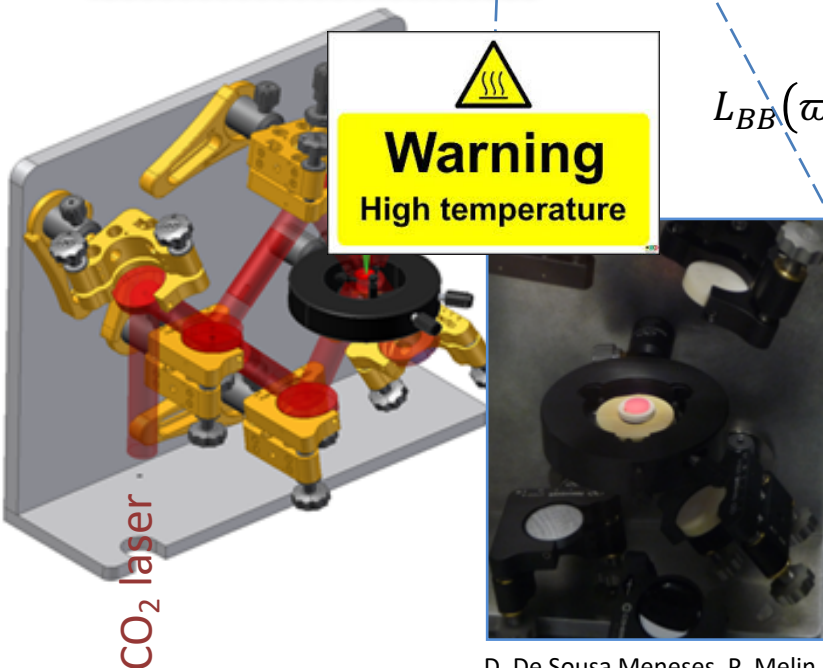
* Measurement at near-normal incidence

Emittance measurement

$$L_{BB}(\varpi, \hat{T}) \quad L(\varpi, \hat{T}, \theta)$$



Blackbody reference

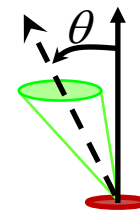


CO₂ laser

Directional spectral emittance measurement

Ratio of the intensities emitted by the sample and a blackbody in the same conditions

$$E(\varpi, \hat{T}, \theta) = \frac{L(\varpi, \hat{T}, \theta)}{L_{BB}(\varpi, \hat{T})}$$



\hat{T} : temperature

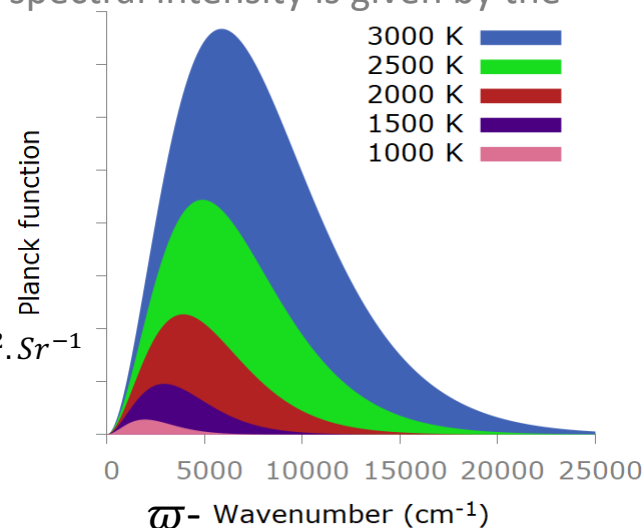
Blackbody

Ideal radiator whose spectral intensity is given by the Planck's law

$$L_{BB}(\varpi, \hat{T}) = \frac{C_1 \varpi^3}{\exp\left(\frac{C_2 \varpi}{\hat{T}}\right) - 1}$$

$$C_1 = 1,191043 \cdot 10^{-16} \text{ W.m}^2 \cdot \text{Sr}^{-1}$$

$$C_2 = 0,01438777 \text{ mK}$$



Kirchhoff's law

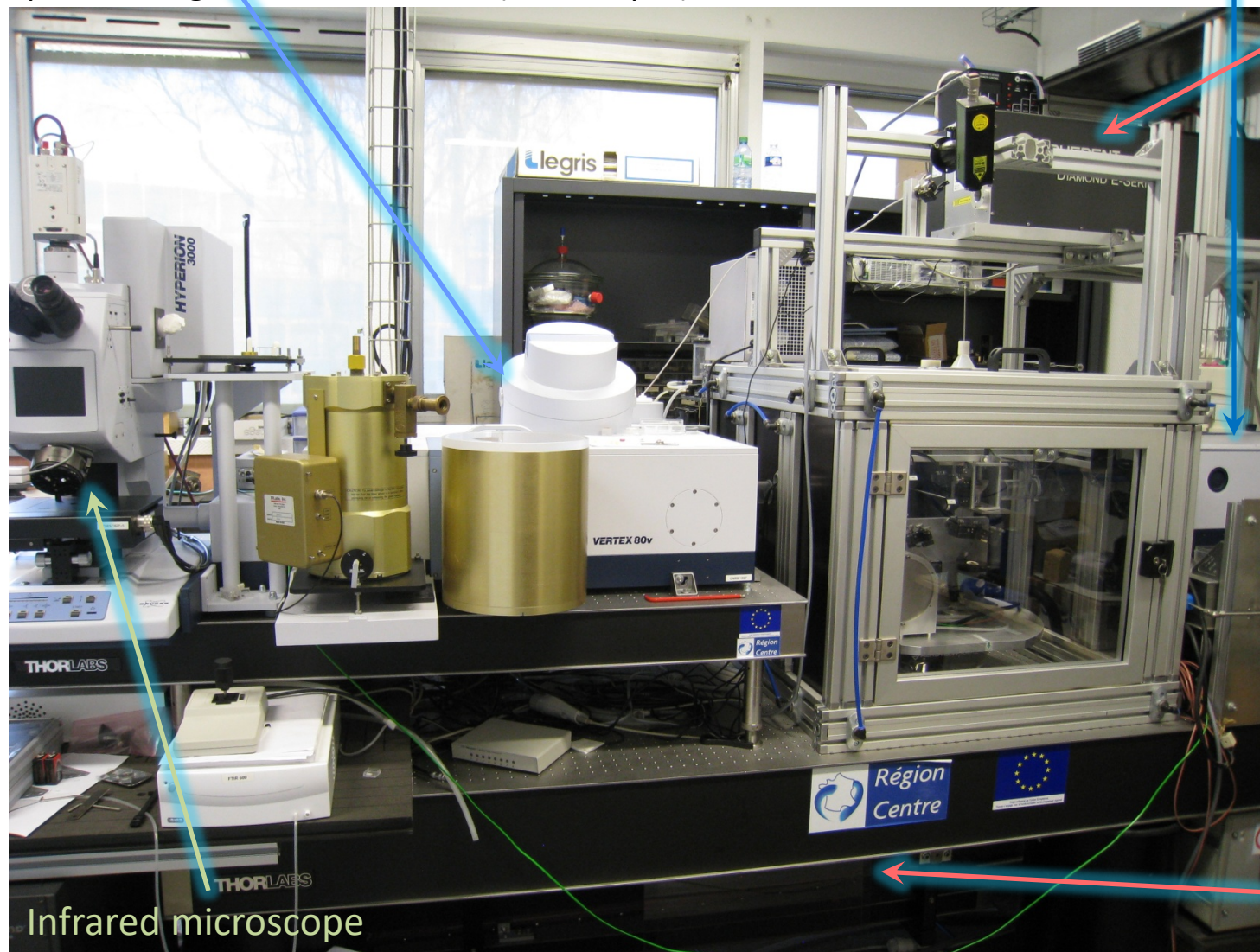
At LTE, spectral absorptance A and emittance are equal

$$A(\varpi) = E(\varpi)$$

Infrared emission spectrometer

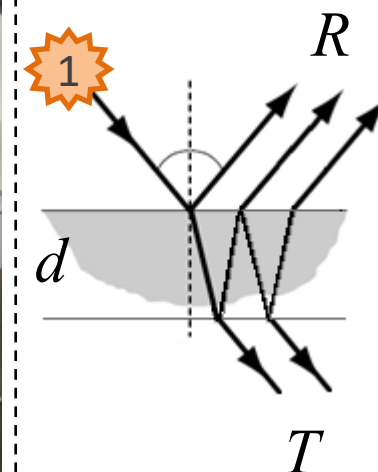
Bruker Vertex 80v and Vertex 70

Spectral range: $[20-20\,000\text{ cm}^{-1}]$ ($500-0.5\ \mu\text{m}$)



CO₂ laser (500W)
[400 - 3000 K]

Measurements
Reflection R
Transmission T



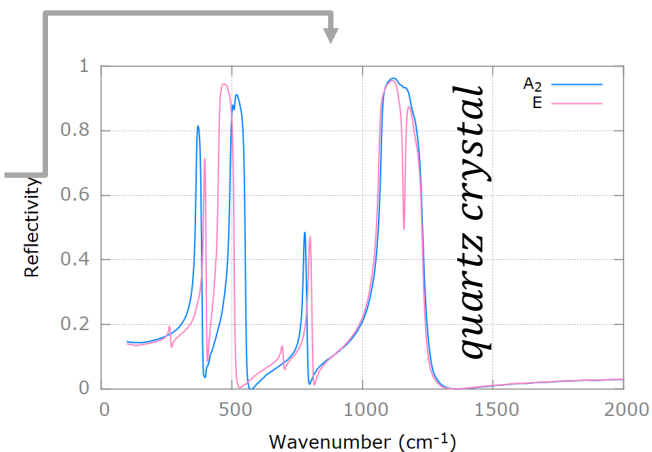
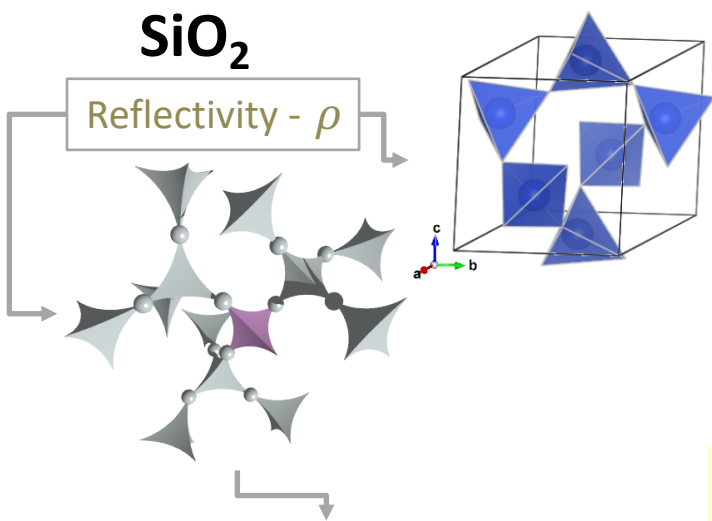
Emission E

CO₂ laser (500W)
[400 - 3000 K]

Infrared microscope

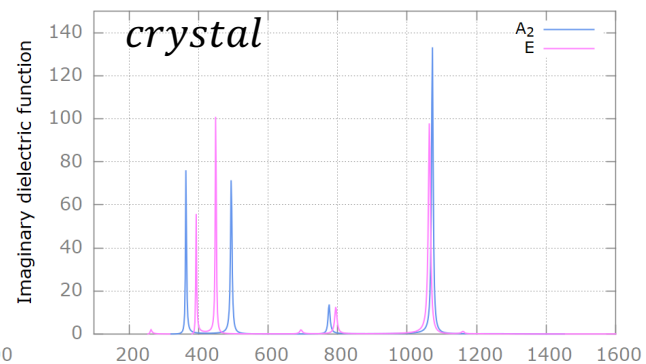
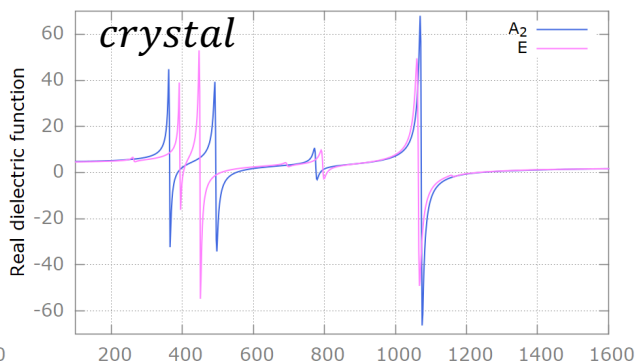
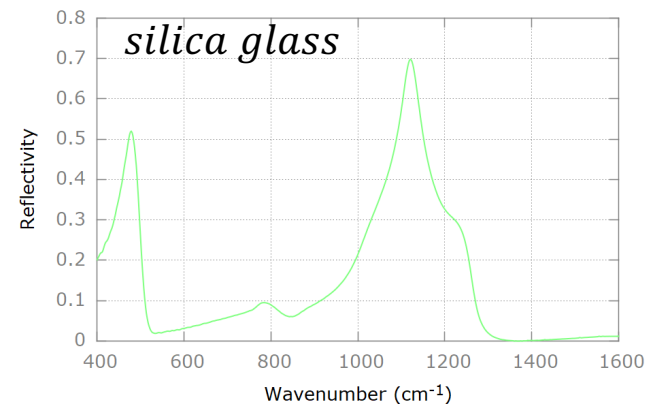
D. De Sousa Meneses, P. Melin, L. del Campo, L. Cosson, P. Echegut Infrared Physics & Technology 69 96–101 2015

Infrared spectroscopy



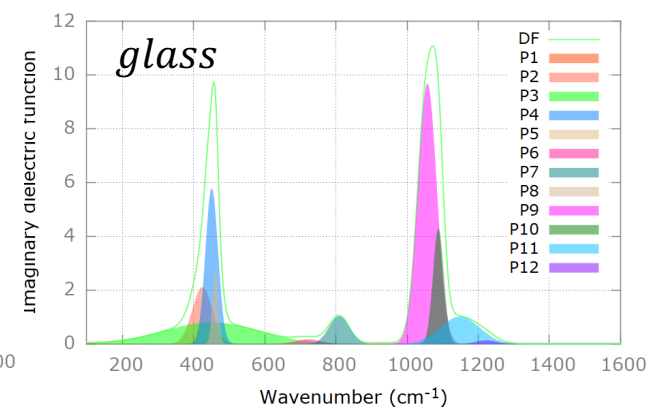
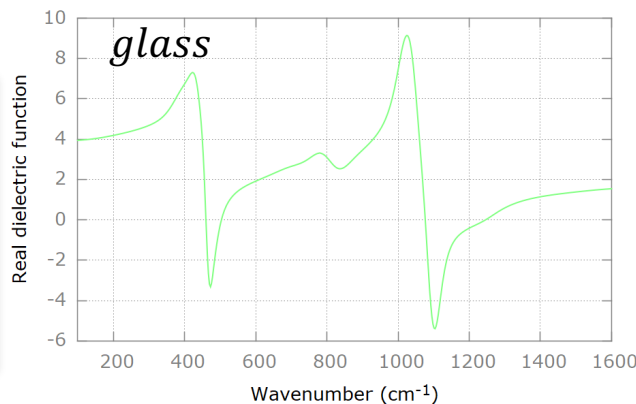
Single crystal
Anisotropic infrared response.
Activity of normal modes (phonons) fixed by crystal symmetry and infrared spectroscopy selection rules

From experimental observables to physical properties



Glass

Isotropic infrared response.
The complexity of the glass structure is revealed by its polar vibrational dynamics.



Complex refractive index extraction – inversion methods

IR-Visible-UV spectroscopies Ellipsometry

	R_p	R_s	ρ	R_M	T_M	E	ψ	Δ
R_p								
R_s								
ρ								
R_M								
T_M								
E								
ψ								
Δ								

Several inversion methods necessitates the knowledge of two experimental quantities.

Under certain conditions, 1 measure may be sufficient to determine the indices

Semi-transparent media

$$\begin{matrix} R_M \\ T_M \end{matrix}$$

$$\begin{matrix} R_M \\ E \end{matrix}$$

$$T_M = 1 - R_M - E$$

$$\begin{matrix} T_M \\ E \end{matrix}$$

$$R_M = 1 - T_M - E$$

$$\rho = \frac{R_M(R_M - 2) - T_M^2 - 1 + \sqrt{[1 + T_M^2 - R_M(R_M - 2)]^2 + 4R_M(R_M - 2)}}{2(R_M - 2)}$$

$$\tau = \frac{1}{T_M} \left(\frac{R_M}{\rho} - 1 \right)$$



$$n(\omega) = \frac{1 + \rho(\omega) + \sqrt{4\rho(\omega) - (\rho(\omega) - 1)^2 k(\omega)^2}}{1 - \rho(\omega)}$$

$$k(\omega) = -\frac{\ln(\tau(\omega))}{4\pi\omega d}$$

Semi-infinite media

$$\psi, \Delta$$

$$n(\omega) + ik(\omega) = \sin(\theta_0) \sqrt{1 + \left[\frac{1 + \tan(\Psi(\omega))e^{i\Delta(\omega)}}{1 - \tan(\Psi(\omega))e^{i\Delta(\omega)}} \right]^2 \tan^2(\theta_0)}$$

θ_0 : angle of incidence

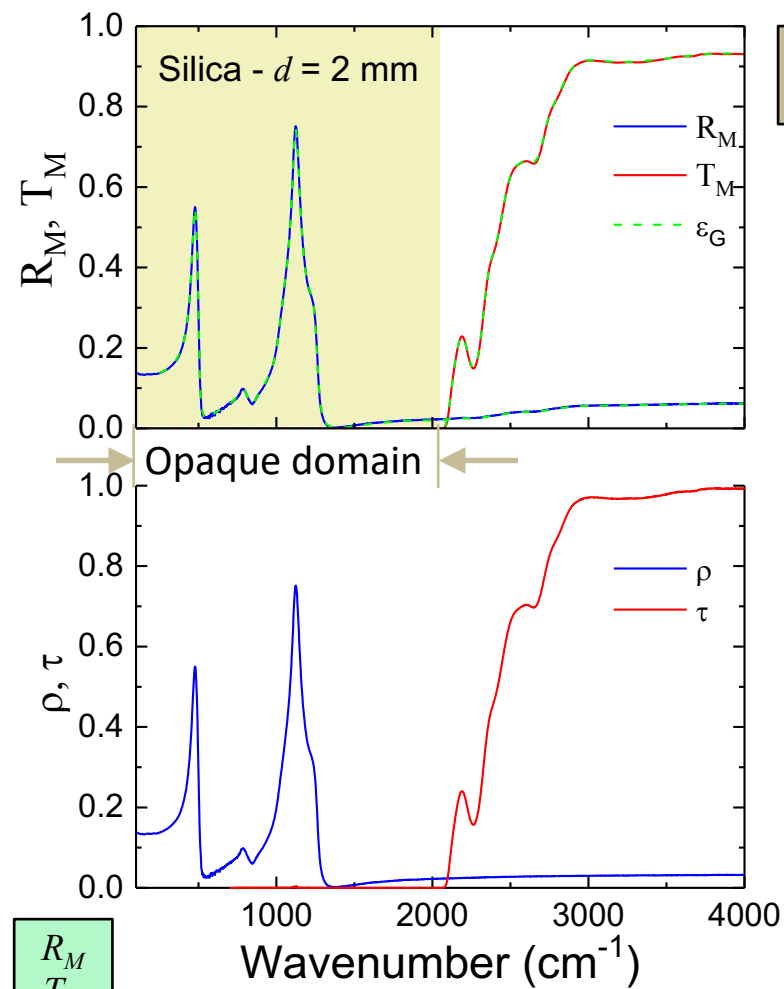
KK Inversion method using the Kramers-Kronig relations

$$\delta(\omega_a) = \frac{1}{2\pi} \int_0^\infty \ln \left| \frac{\omega - \omega_a}{\omega + \omega_a} \right| \frac{d}{d\omega} \ln[\rho(\omega)] d\omega \quad n(\omega) = \frac{1 - \rho(\omega)}{1 + \rho(\omega) - 2\sqrt{\rho(\omega)} \cdot \cos[\delta(\omega)]} \quad k(\omega) = \frac{2\sqrt{\rho(\omega)} \cdot \sin[\delta(\omega)]}{1 + \rho(\omega) - 2\sqrt{\rho(\omega)} \cdot \cos[\delta(\omega)]}$$

D. De Sousa Meneses, J-F. Brun, P. Echegut, P. Simon Applied Spectroscopy 58 (2004) 969-974

Kramers-Kronig Relations in Optical Materials Research, Lucarini, V., Saarinen, J.J., Peiponen, K.-E., Vartiainen, E.M. Springer Series in Optical Sciences, Vol. 110 (2005)

Complex refractive index extraction – inversion methods



KK

$$\delta(\omega_a) = \frac{1}{2\pi} \int_0^\infty \ln \left| \frac{\omega - \omega_a}{\omega + \omega_a} \right| \frac{d}{d\omega} \ln[\rho(\omega)] d\omega$$

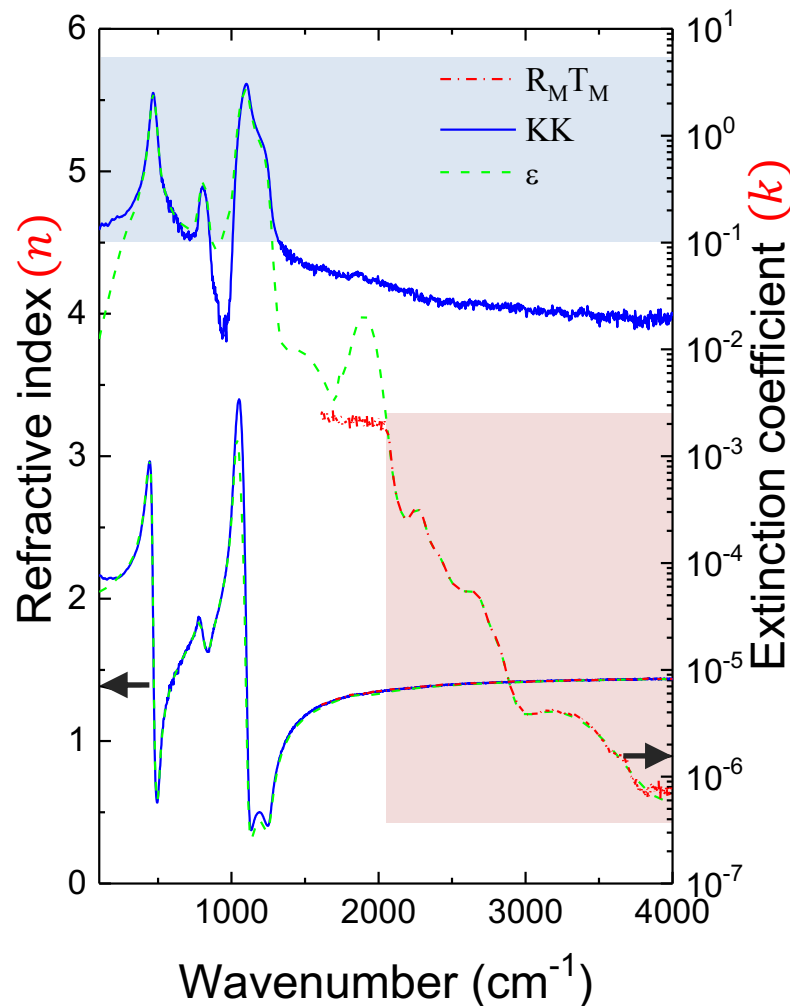
$$n(\omega) = \frac{1 - \rho(\omega)}{1 + \rho(\omega) - 2\sqrt{\rho(\omega)} \cdot \cos[\delta(\omega)]} \quad k(\omega) = \frac{2\sqrt{\rho(\omega)} \cdot \sin[\delta(\omega)]}{1 + \rho(\omega) - 2\sqrt{\rho(\omega)} \cdot \cos[\delta(\omega)]}$$

R_M
 T_M

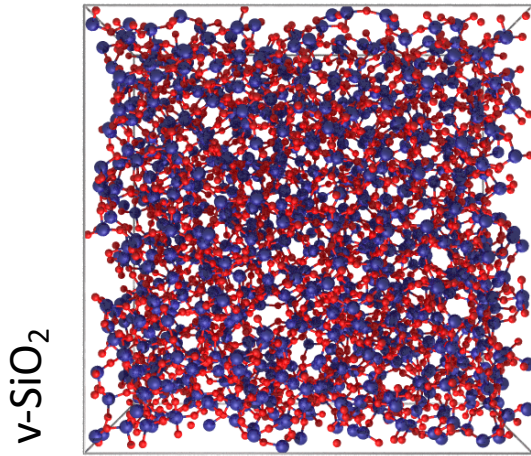
$$\rho = \frac{R_M(R_M - 2) - T_M^2 - 1 + \sqrt{[1 + T_M^2 - R_M(R_M - 2)]^2 + 4R_M(R_M - 2)}}{2(R_M - 2)}$$

$$\tau = \frac{1}{T_M} \left(\frac{R_M}{\rho} - 1 \right)$$

$$n(\omega) = \frac{1 + \rho(\omega) + \sqrt{4\rho(\omega) - (\rho(\omega) - 1)^2 k(\omega)^2}}{1 - \rho(\omega)} \quad k(\omega) = -\frac{\ln(\tau(\omega))}{4\pi\omega d}$$



Dielectric function models – disordered media

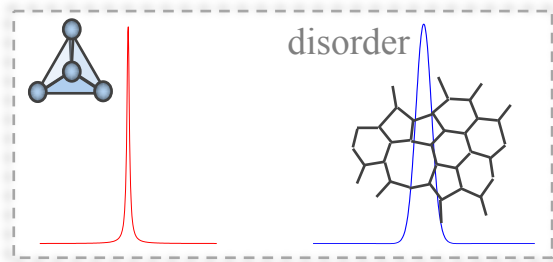


Lorentz model

Single crystals

$$\varepsilon(\omega) = \varepsilon_{\infty} + \sum_j \frac{S_j \omega_j^2}{\omega_j^2 - \omega^2 - i\gamma_j \omega}$$

The Lorentz dielectric function model (DHO - Damped Harmonic Oscillator) used for the adjustment of crystal spectra is not suitable for glasses.



Causal Voigt model

Allows to account for a Gaussian (G) broadening of a Lorentzian absorption profile (L).

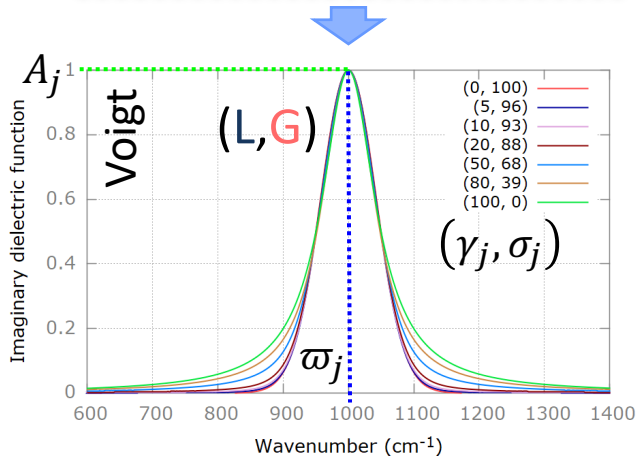
$$\varepsilon_V(\omega) = \varepsilon_{\infty} + \sum_j \hat{V}_j(\omega) = \varepsilon_{\infty} + \sum_j \hat{V}(\omega; A_j, \omega_j, \gamma_j, \sigma_j)$$

$$\hat{V}_j(\omega) = \hat{V}_j(x, y)$$

$$= A_j \left[-\frac{\Im(w(x - x_j + iy) + w(x + x_j + iy))}{\Re(w(iy))} + i \frac{\Re(w(x - x_j + iy) - w(x + x_j + iy))}{\Re(w(iy))} \right]$$

$$x = \frac{2\sqrt{\ln 2}}{\sigma_j} \omega \quad x_j = \frac{2\sqrt{\ln 2}}{\sigma_j} \omega_j \quad y = \frac{\gamma_j}{\sigma_j} \sqrt{\ln 2}$$

$$\text{Faddeeva function: } w(z) = \frac{i}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-t^2}}{z - t} dt = K(x, y) + iJ(x, y)$$



D. De Sousa Meneses et al. J. Non-Cryst. Solids 351 (2005) 124-129.

Dielectric function models – disordered media

Convolution model

Expression based on a Gaussian distribution of damped harmonic oscillators

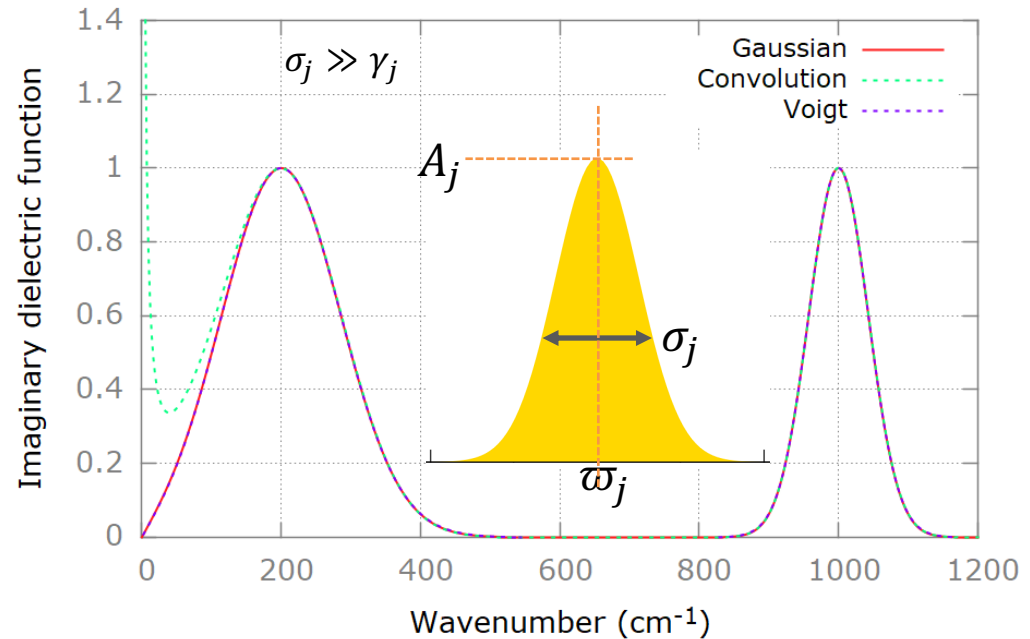
$$\varepsilon(\omega) = \varepsilon_{\infty} + \sum_j \frac{S_j}{\sqrt{2\pi}\sigma_j} \int_{-\infty}^{+\infty} \frac{\exp\left[-\frac{1}{2}\left(\frac{x - \omega_j}{\sigma_j}\right)^2\right]}{x^2 - \omega^2 - i\gamma_j\omega} dx$$

H. Hobert, H. H. Dunken J. Non-Cryst. Solids 195 (1996) 64-71

A. M. Efimov, J. Non-Cryst. Solids 203 (1996) 1.

T. G. Mayerhofer et al. J. Non-Cryst. Solids 333 (2004) 172–181.

The Voigt and convolution models have close absorption profiles for high frequency modes with low inhomogeneous broadening. The difference can be large at low frequency.



Causal Gaussian model

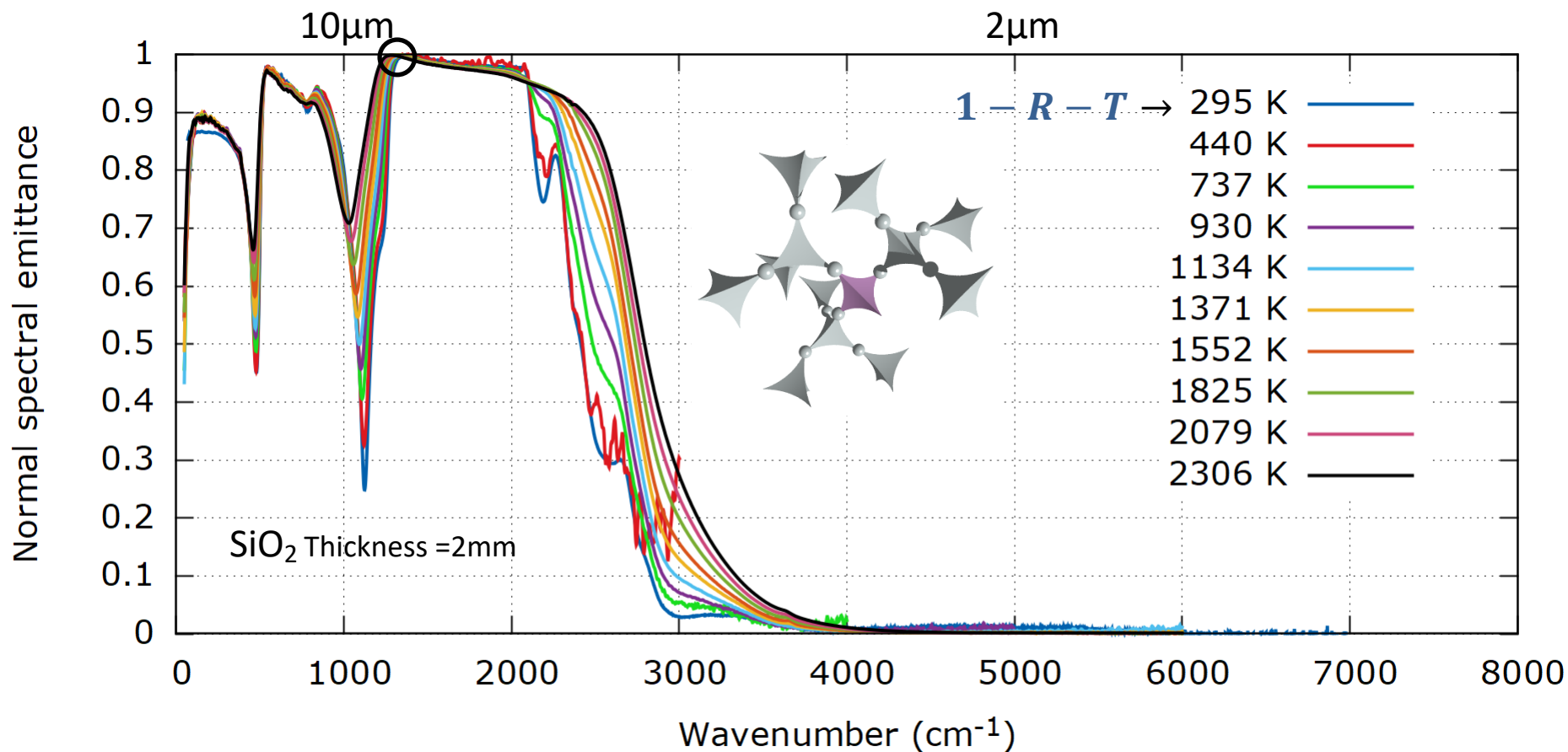
Allows to take into account several components having a Gaussian absorption profile respecting the causality principle.

$$\varepsilon(\omega) = \varepsilon_{\infty} + \sum_j \frac{2A_j}{\sqrt{\pi}} \left[D\left(2\sqrt{\ln 2} \frac{\omega + \omega_j}{\sigma_j}\right) - D\left(2\sqrt{\ln 2} \frac{\omega - \omega_j}{\sigma_j}\right) \right] + i A_j \left[\exp\left(-4\ln 2 \left(\frac{\omega - \omega_j}{\sigma_j}\right)^2\right) - \exp\left(-4\ln 2 \left(\frac{\omega + \omega_j}{\sigma_j}\right)^2\right) \right]$$

Dawson function: $D(x) = \exp(-x^2) \int_0^x \exp(t^2) dt$

D. De Sousa Meneses, M. Malki, P. Echegut, J. Non-Cryst. Solids 351 (2006) 769-776.

Normal spectral emittance of a silica glass



Temperature measurement at the Christiansen point \bigcirc $n = 1, k \ll 1 \rightarrow E \cong 1$

Retrieval of the complex refractive index $N(\omega) = n(\omega) + i k(\omega)$

Fit of the data with the following parallel plate model of emittance (E):

$$E = \frac{(1 - \rho)(1 - \tau)}{1 - \rho\tau} \quad \rho = \frac{(n - 1)^2 + k^2}{(n + 1)^2 + k^2} \quad \tau = \exp(-4\pi k\omega d)$$

d : sample thickness

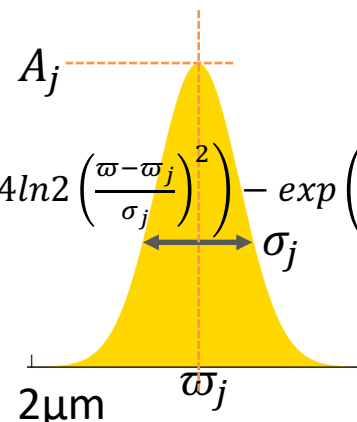
Fit with a dielectric function model

Dielectric function : $\epsilon(\omega) = [N(\omega)]^2$

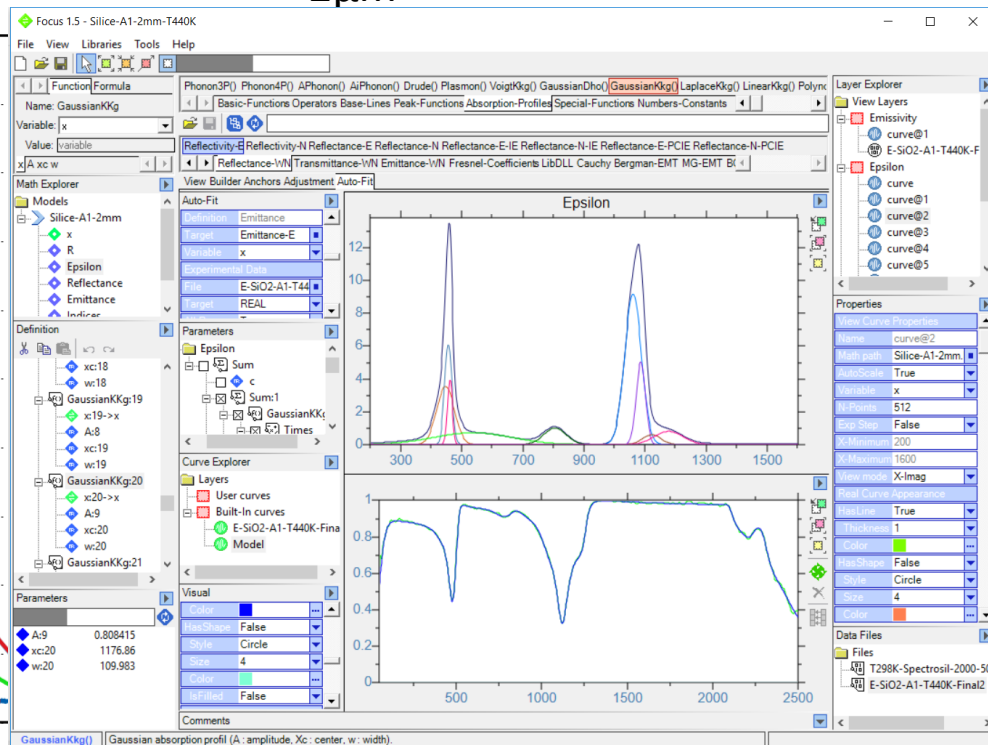
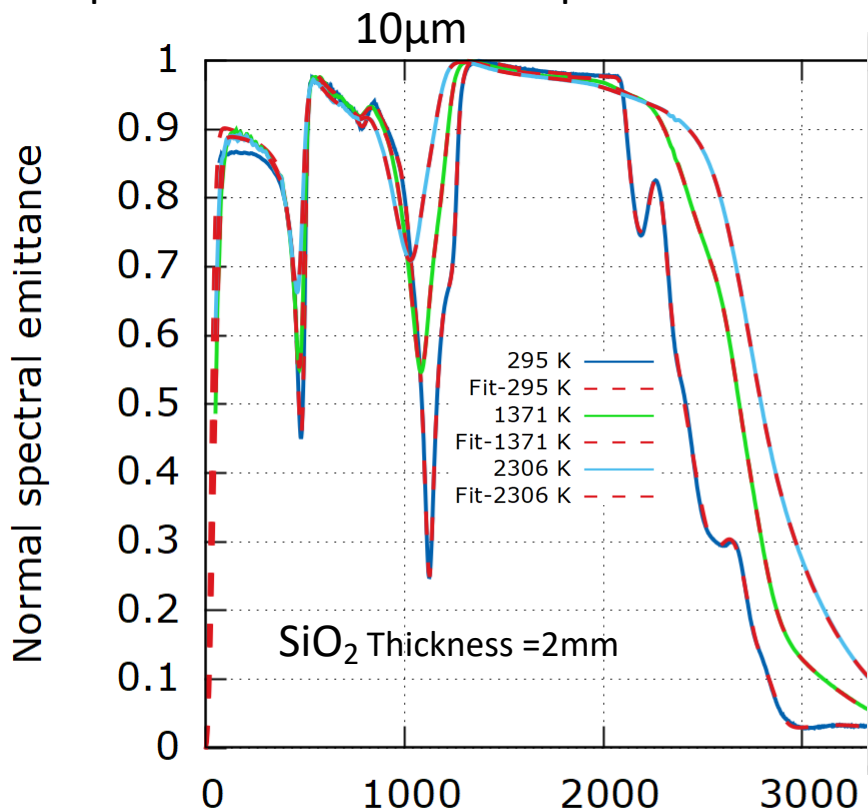
Causal Gaussian dielectric function model for glasses

$$\epsilon(\omega) = \epsilon_{\infty} + \sum_j \frac{2A_j}{\sqrt{\pi}} \left[D \left(2\sqrt{\ln 2} \frac{\omega + \omega_j}{\sigma_j} \right) - D \left(2\sqrt{\ln 2} \frac{\omega - \omega_j}{\sigma_j} \right) \right] + i A_j \left[\exp \left(-4 \ln 2 \left(\frac{\omega - \omega_j}{\sigma_j} \right)^2 \right) - \exp \left(-4 \ln 2 \left(\frac{\omega + \omega_j}{\sigma_j} \right)^2 \right) \right]$$

D is the Dawson function

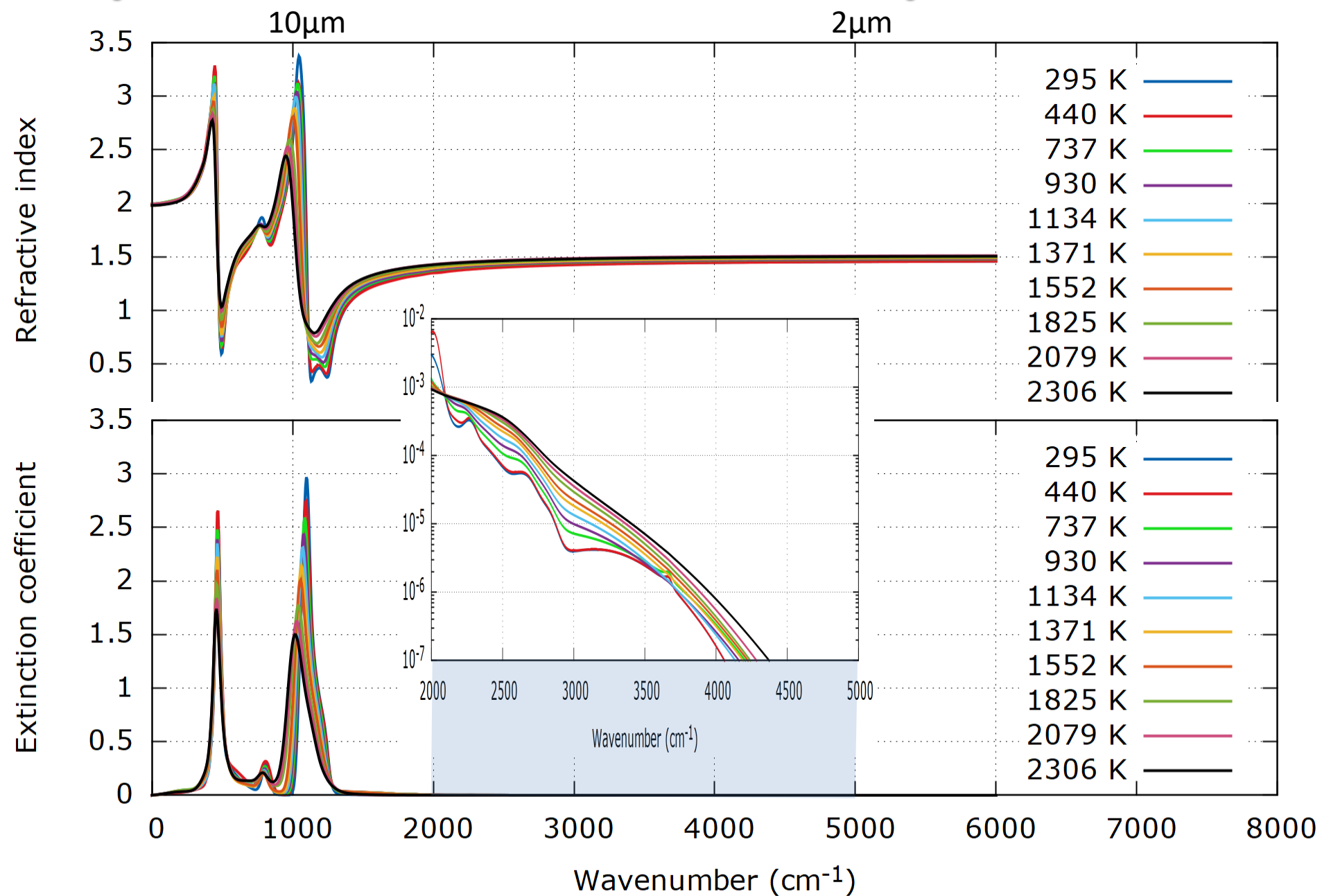


Examples of fit of emittance spectra of a silica glass



Wavenumber (cm⁻¹)

Complex refractive index of the silica sample



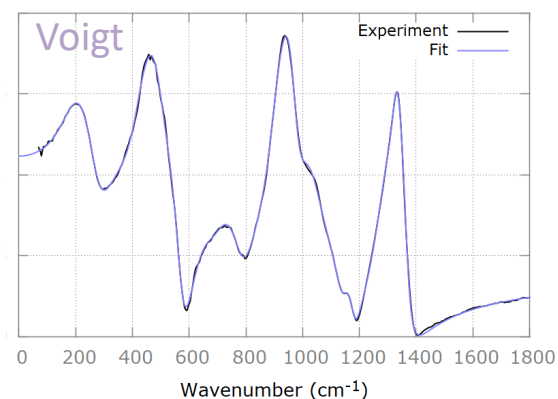
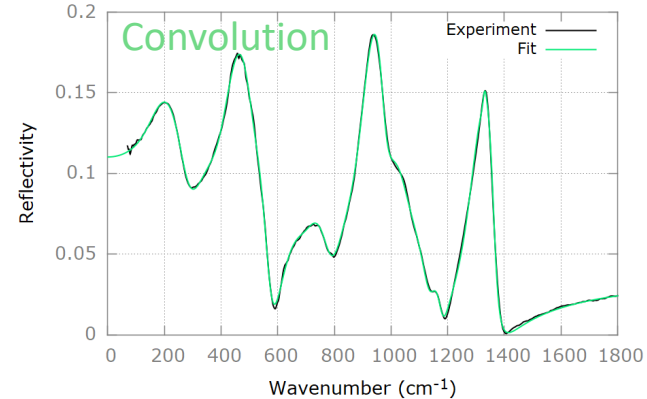
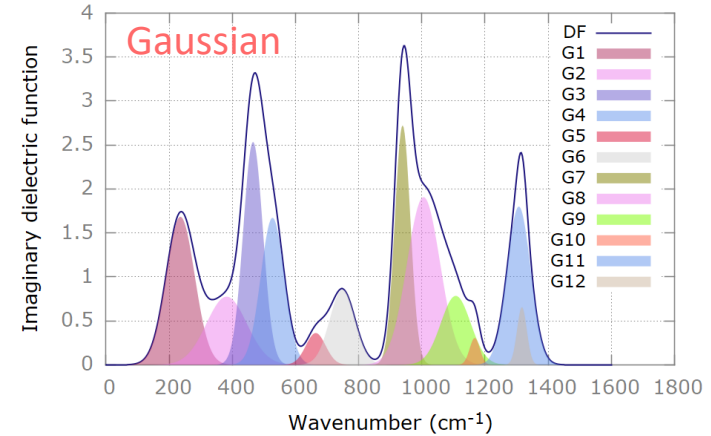
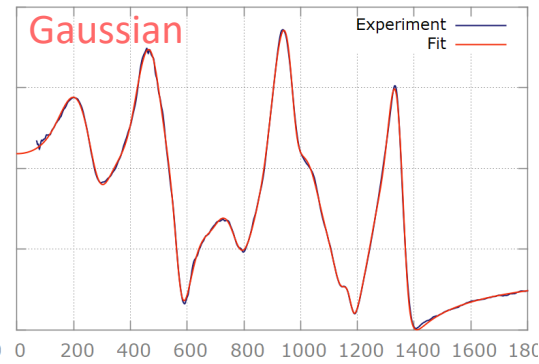
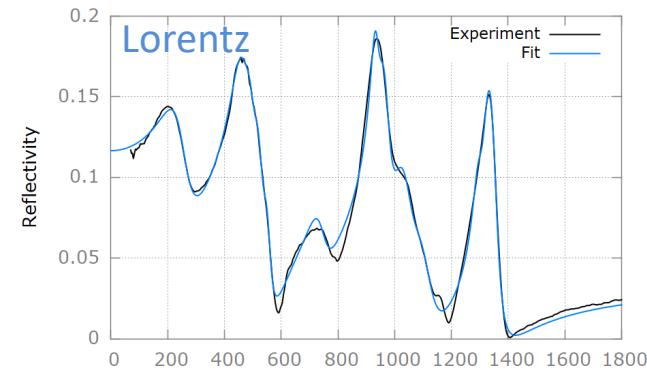
Fit of the reflectivity of a glass with different models

Lorentz model

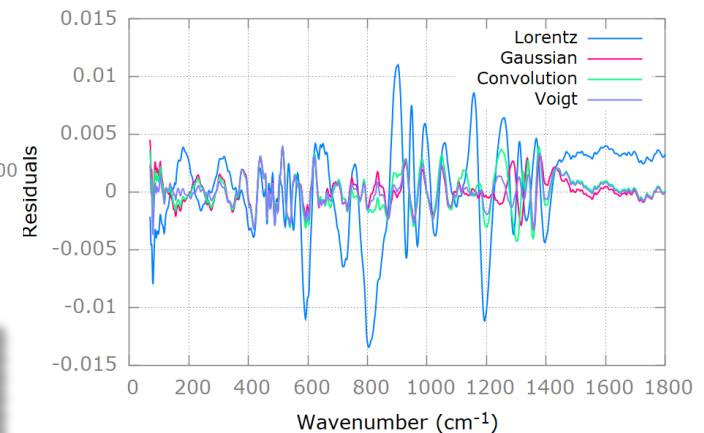
Gaussian model

$(\text{CaO})_x(\text{P}_2\text{O}_5)_{1-x}$ glass

Imaginary dielectric function



Fit residuals



Convolution model

Voigt model

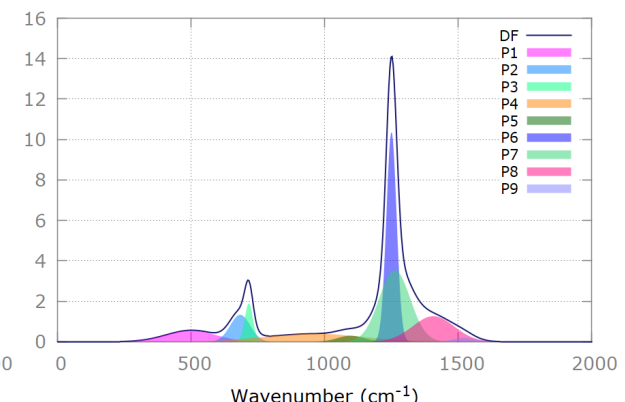
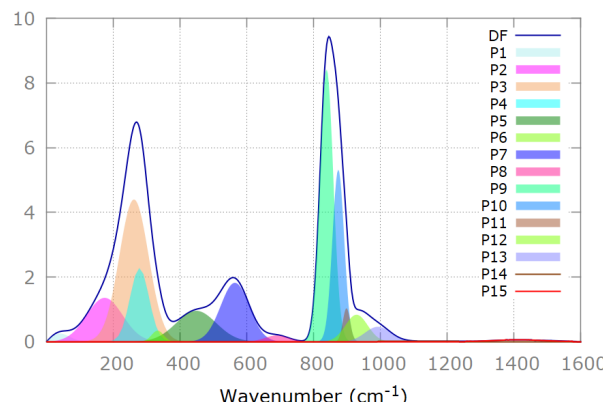
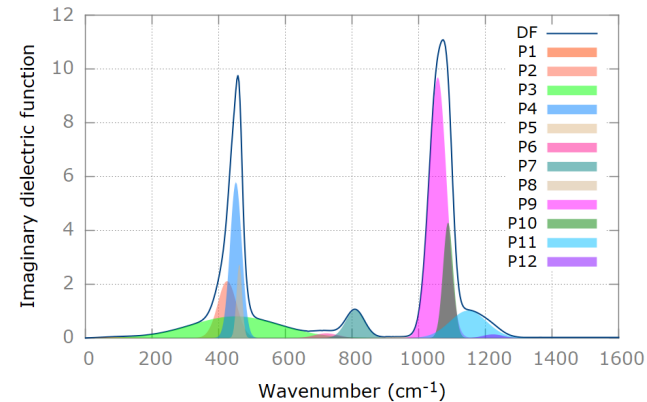
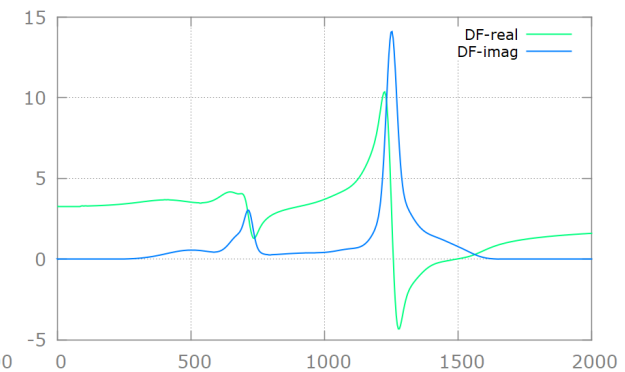
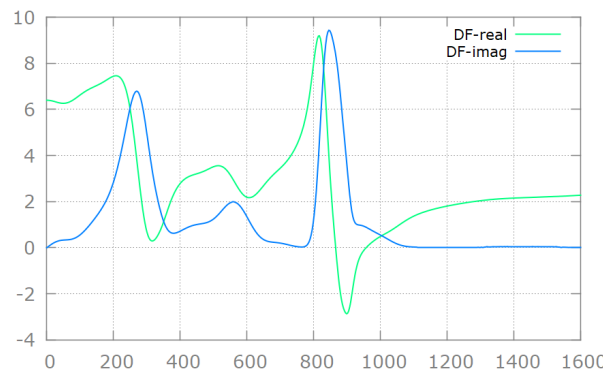
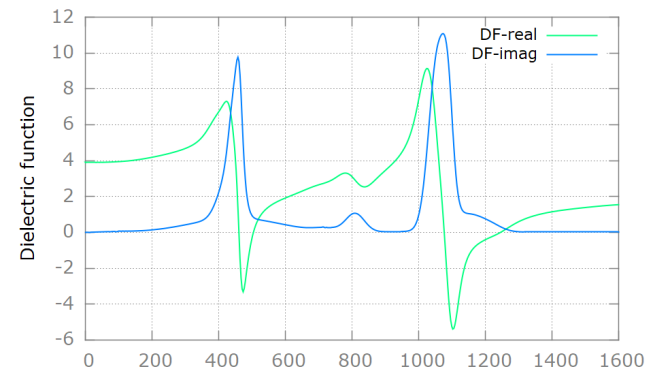
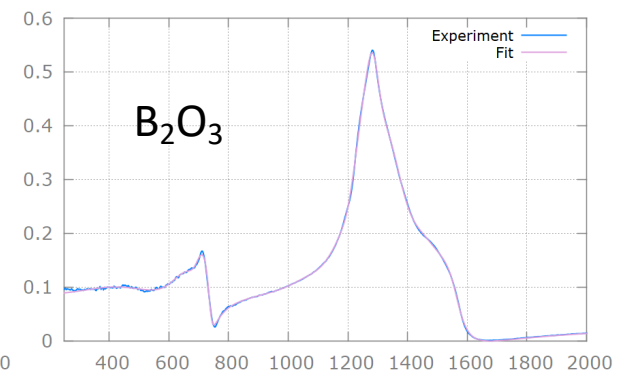
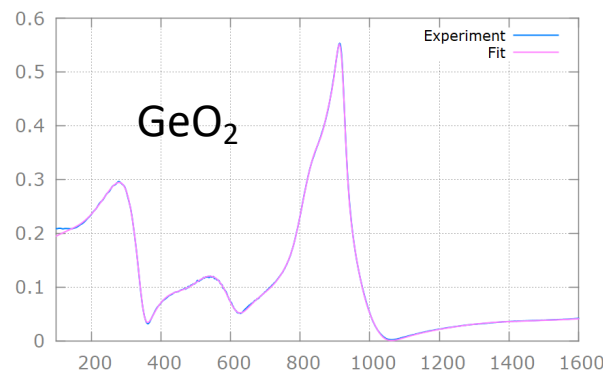
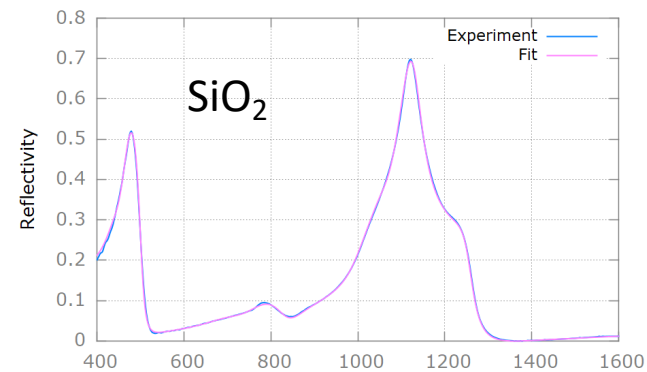
The causal Gaussian dielectric function model represents a good compromise in terms of quality of fit and simplicity for the analysis of the infrared response of most of glasses

Fits of reflectivity with a Gaussian dielectric function model

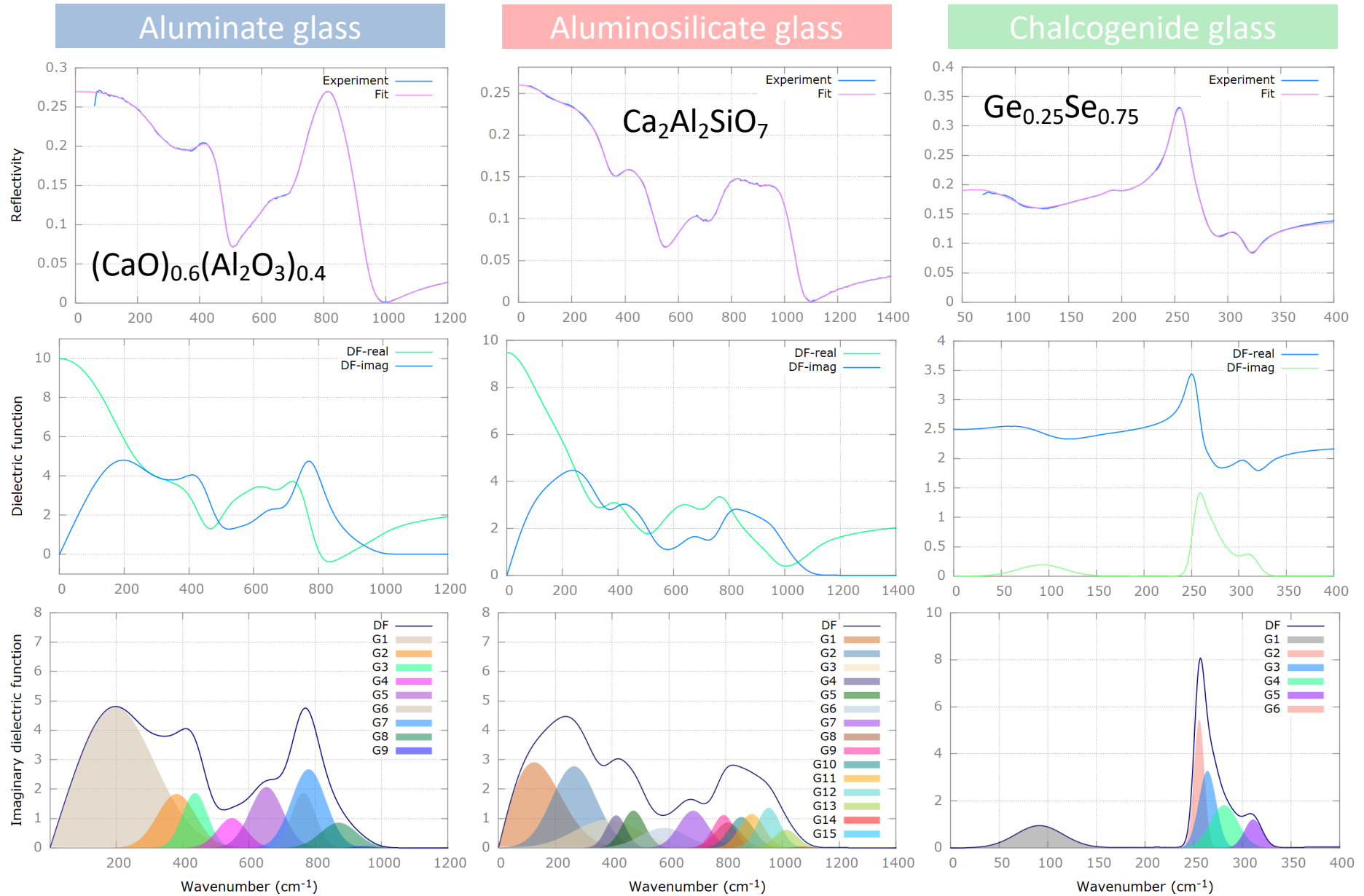
Silica glass

Germania glass

Boria glass



Fits of reflectivity with a Gaussian dielectric function model

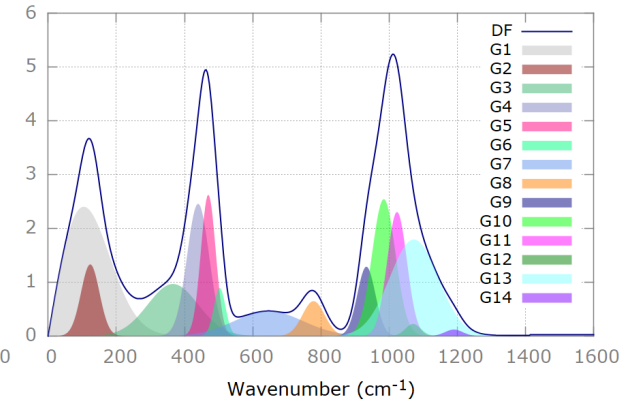
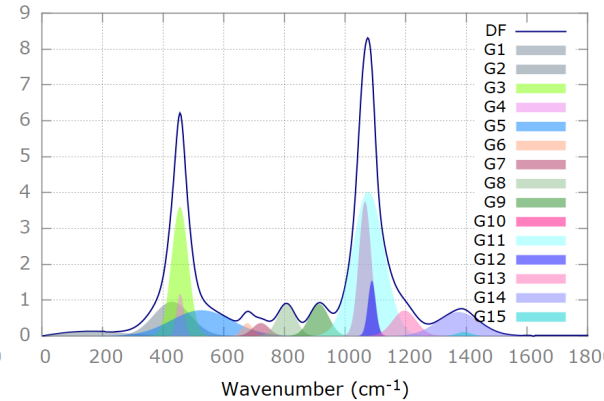
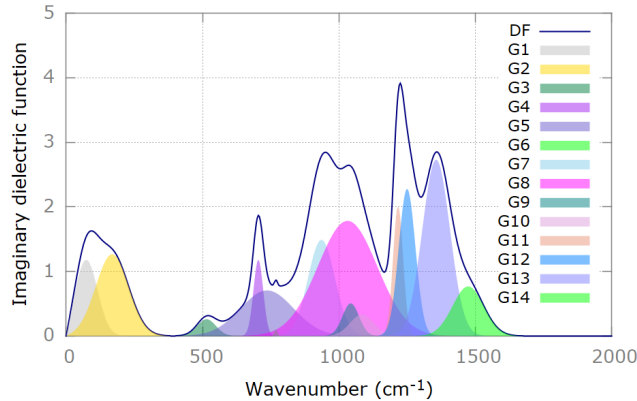
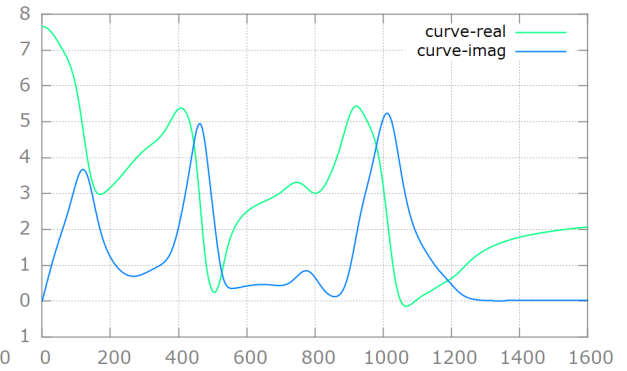
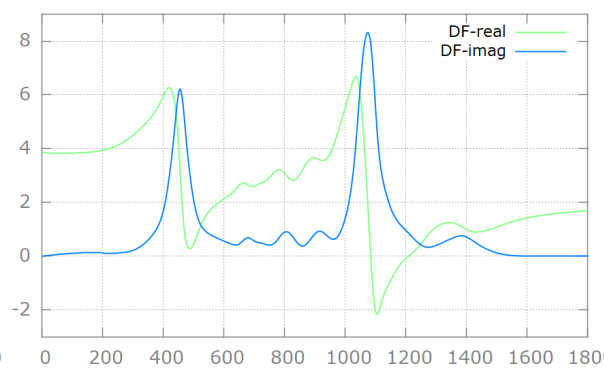
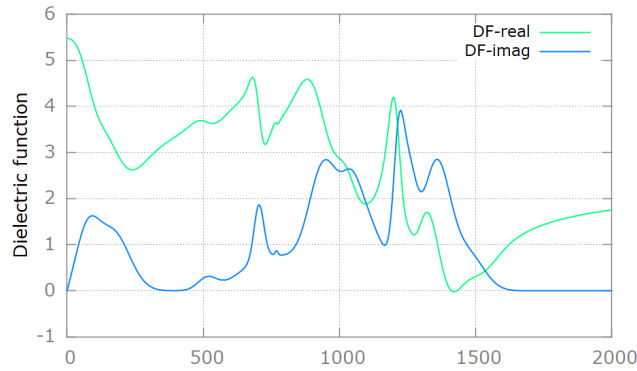
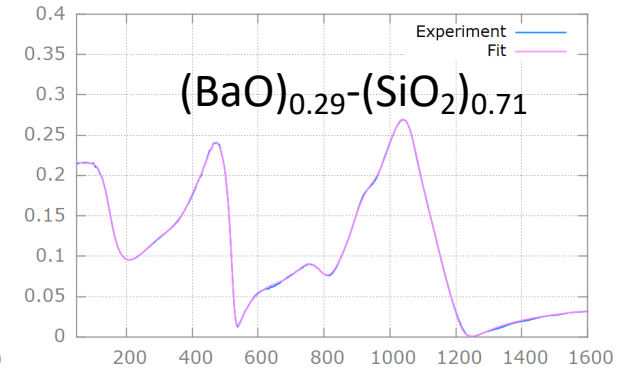
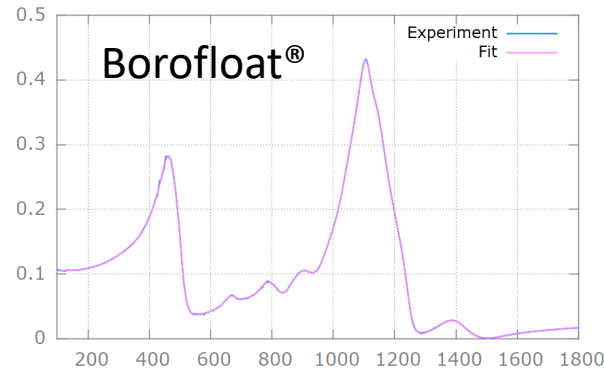
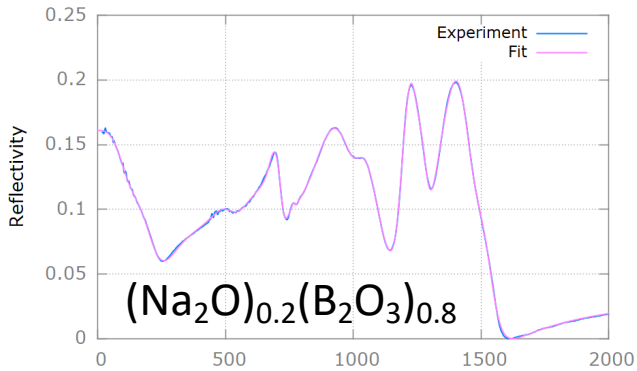


Fits of reflectivity with a Gaussian dielectric function model

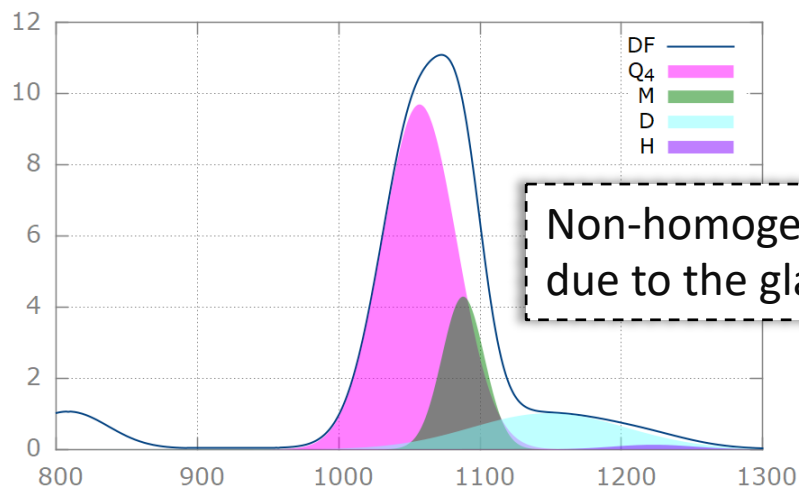
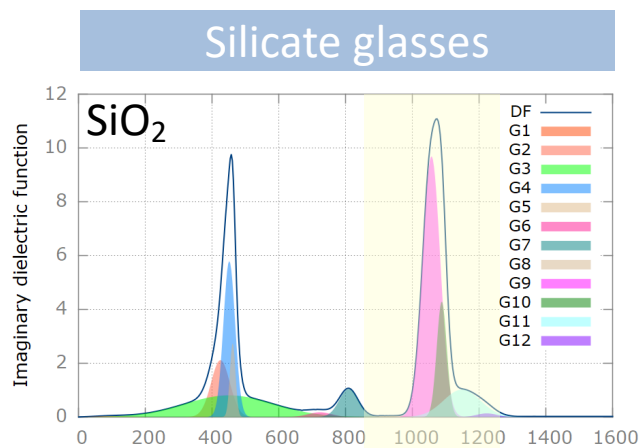
Borate glass

Borosilicate glass

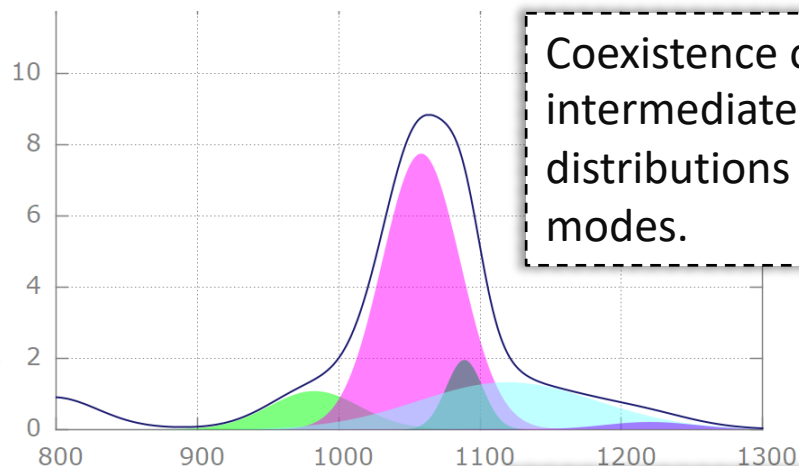
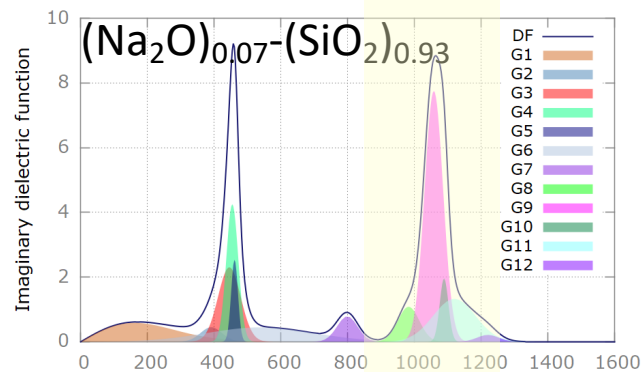
Silicate glass



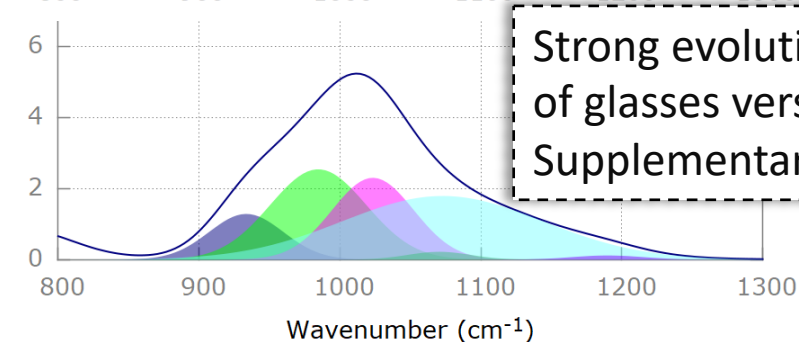
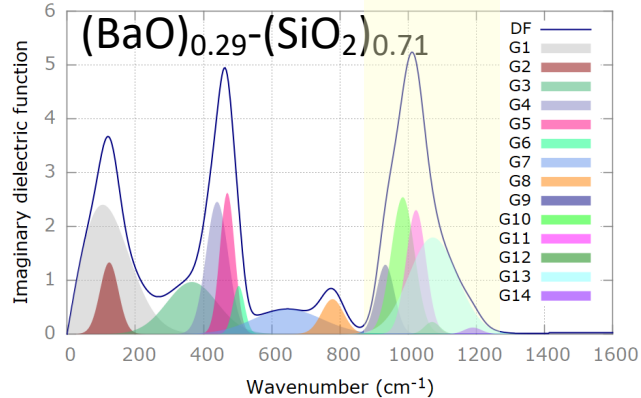
Infrared response of silicate glasses



Non-homogeneous broadening due to the glass disorder.

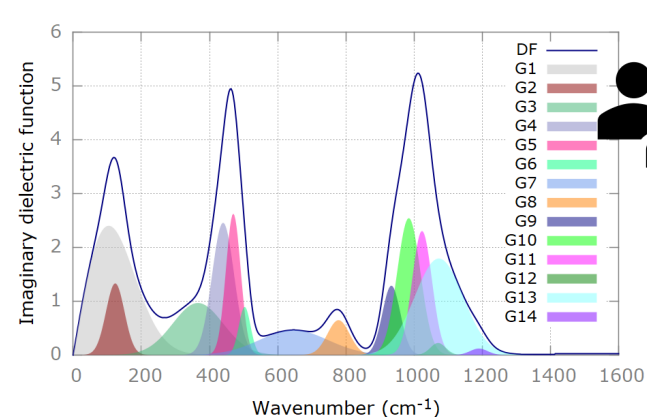


Coexistence of narrow, intermediate and wide distributions of vibrational modes.



Strong evolution of the dynamics of glasses versus composition. Supplementary modes appear.

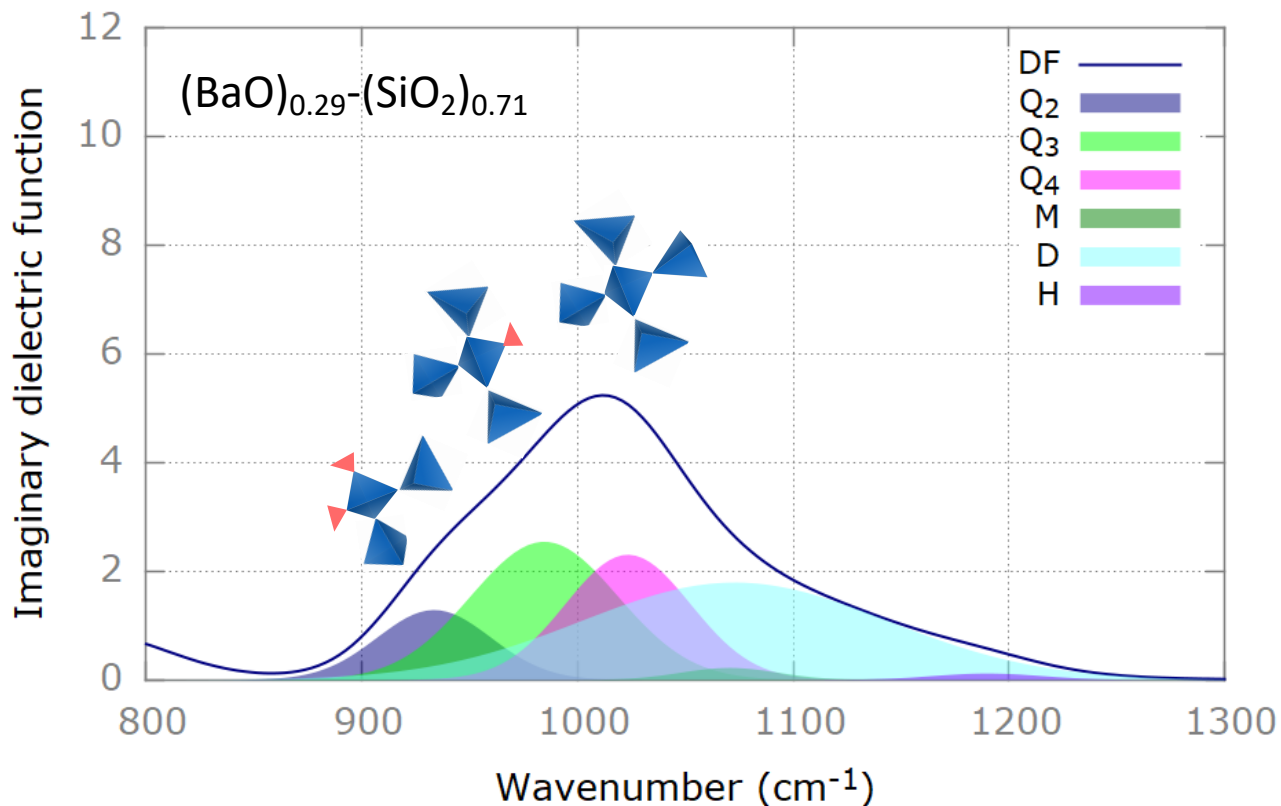
Infrared response of silicate glasses



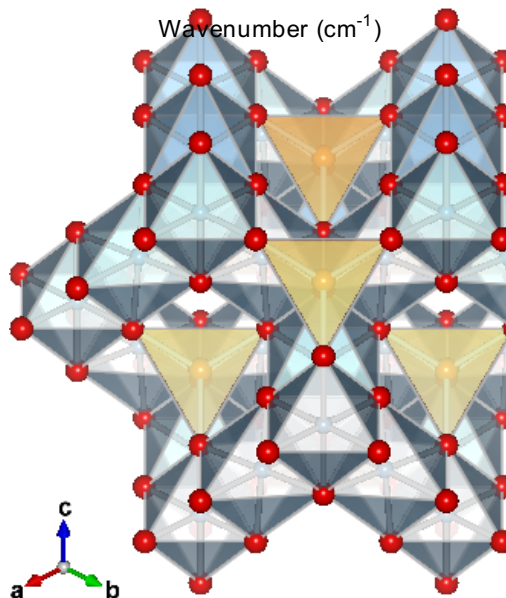
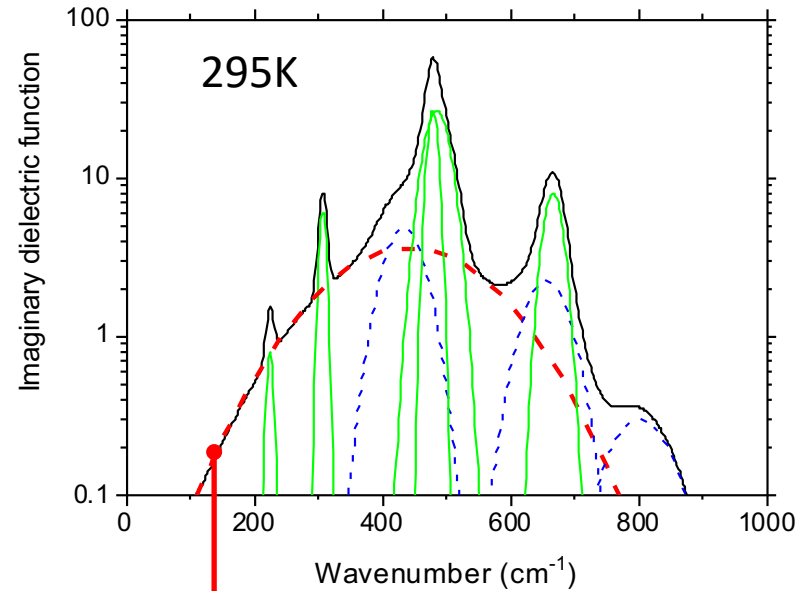
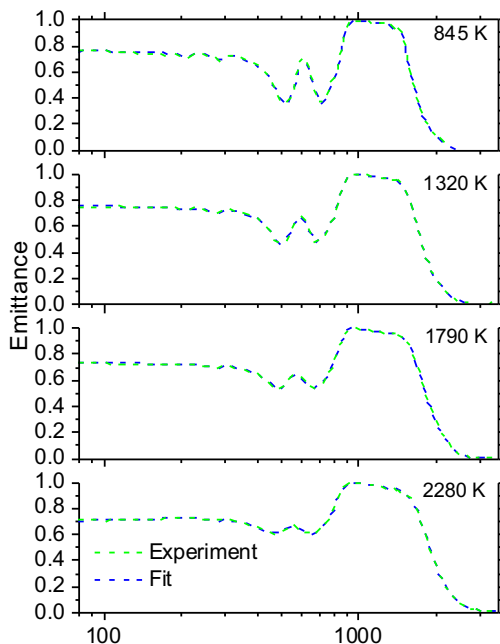
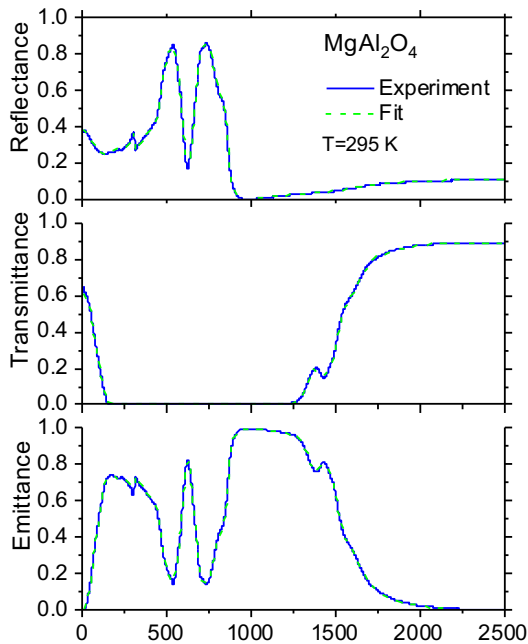
Why such a high number of Gaussian components?
 Do they have a physical meaning?
 What about the fidelity of the dielectric function model?
 Does it include information on the glass network?
 Can I probe cation modifiers?

...

structural disorder
 medium range order
 stretching
 tetrahedral connectivity
 Q_n species
 non bridging oxygen
 local oscillators
 floppy modes
 bridging oxygen
 modifiers
 short range order
 dynamic disorder

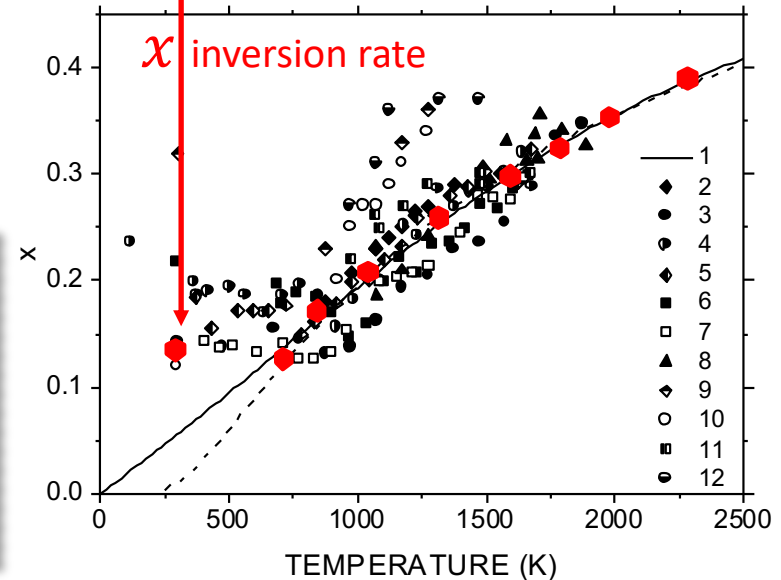


Inversion rate in MgAl_2O_4 versus temperature

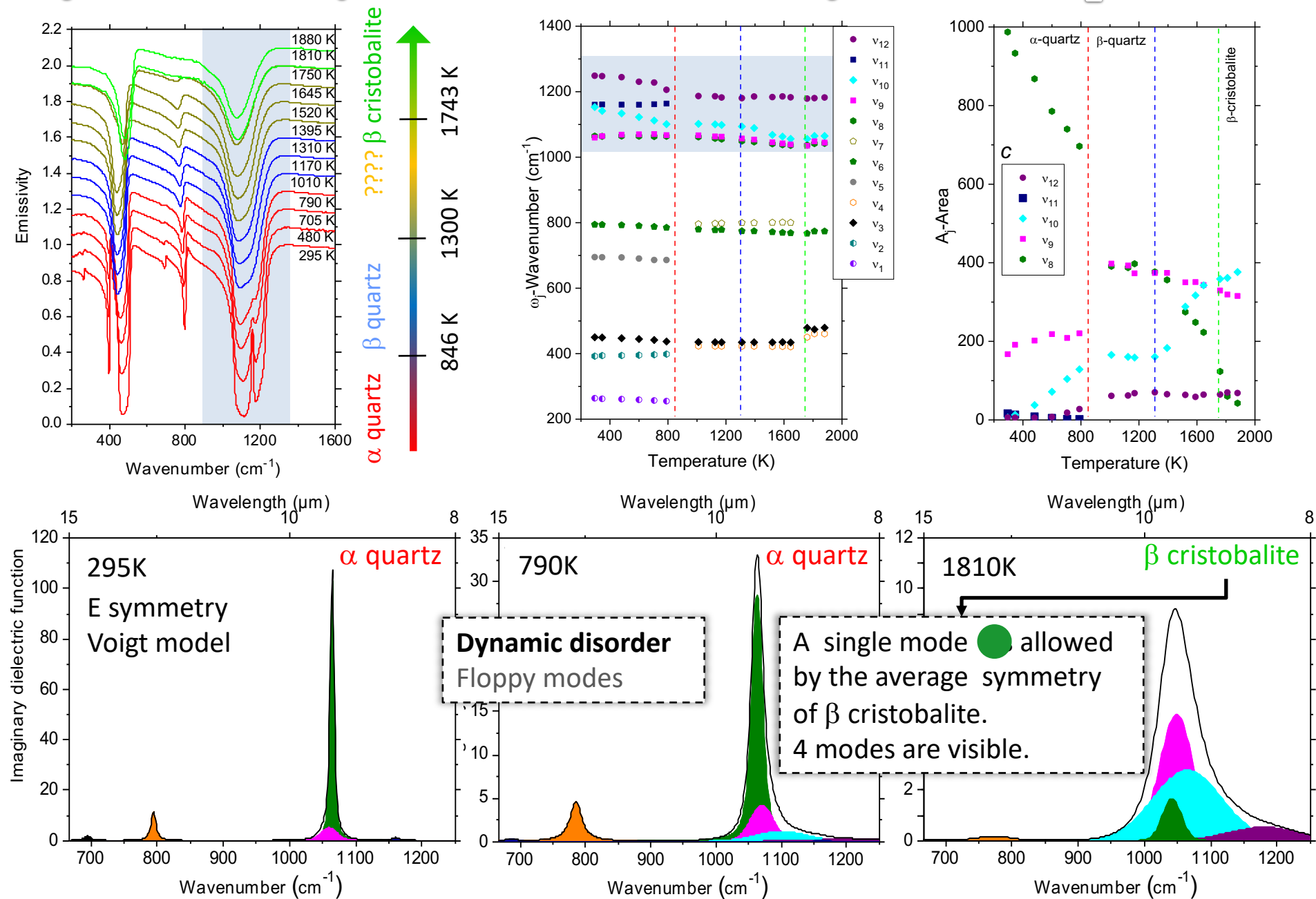


Site occupation disorder
Al/Mg disorder
 $(\text{Mg}_{1-x}\text{Al}_x)[\text{Mg}_x\text{Al}_{2-x}]\text{O}_4$

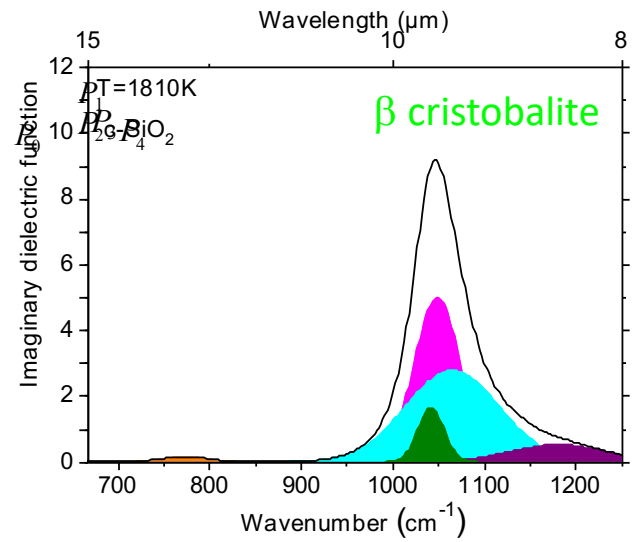
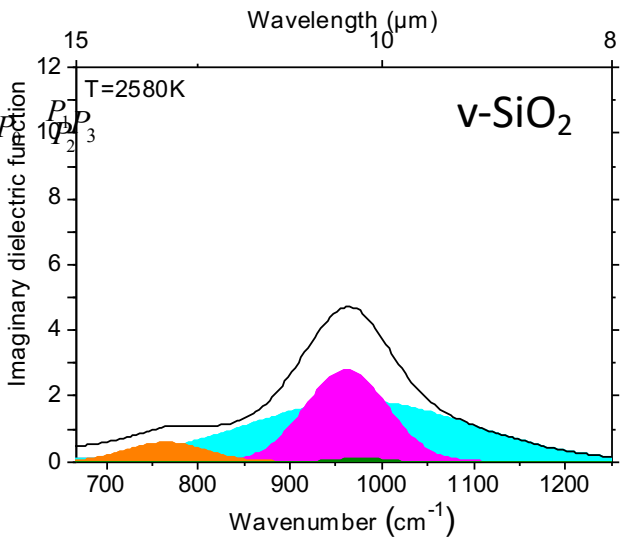
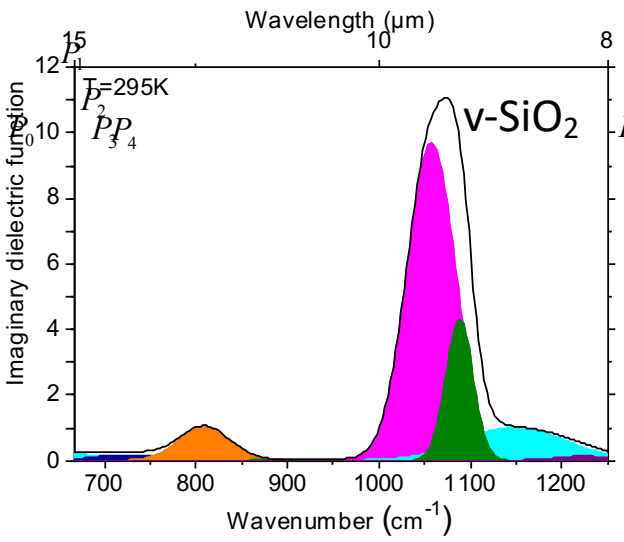
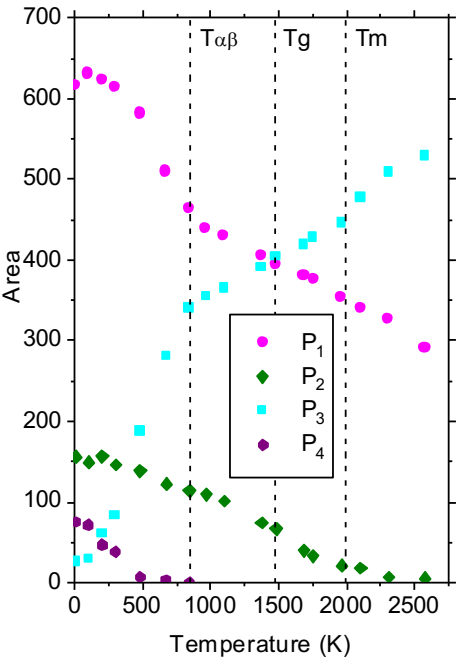
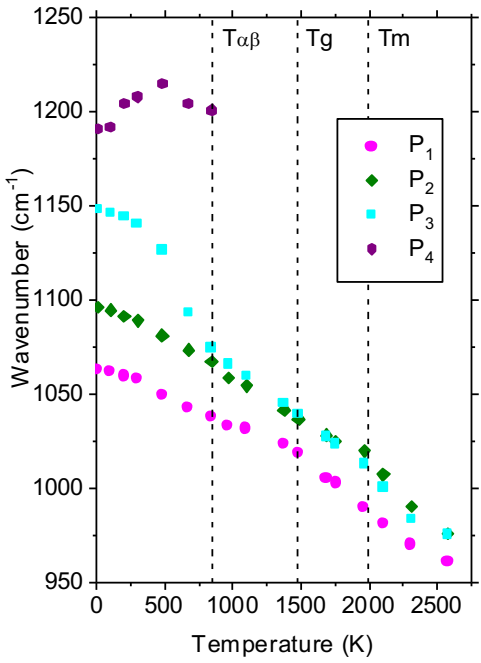
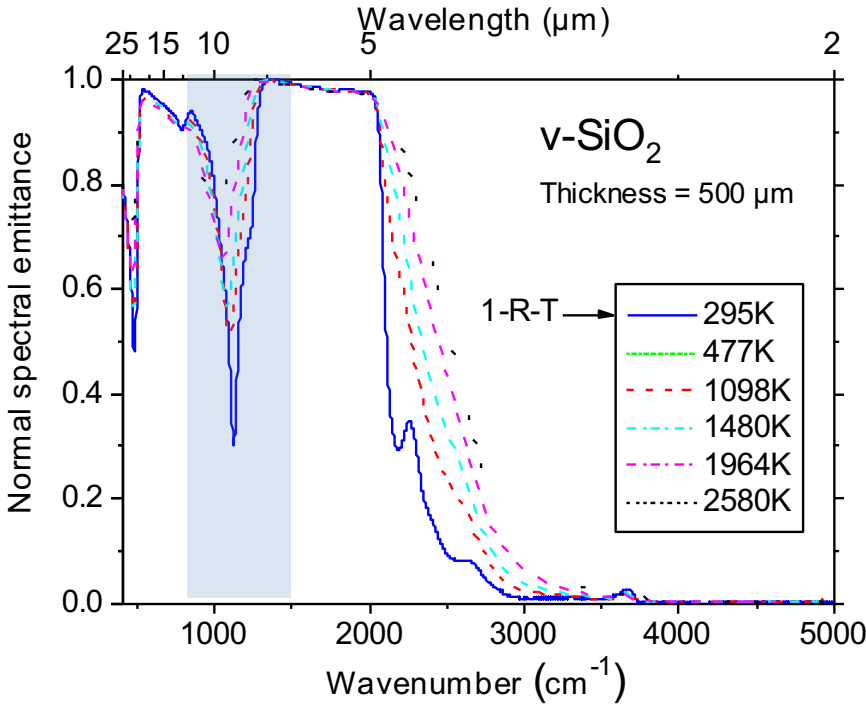
Coexistence of **allowed** modes and modes **forbidden** by symmetry.
Intensity of the **widest** absorption component linked to the inversion rate x .



Dynamics and phase transitions of crystalline SiO₂

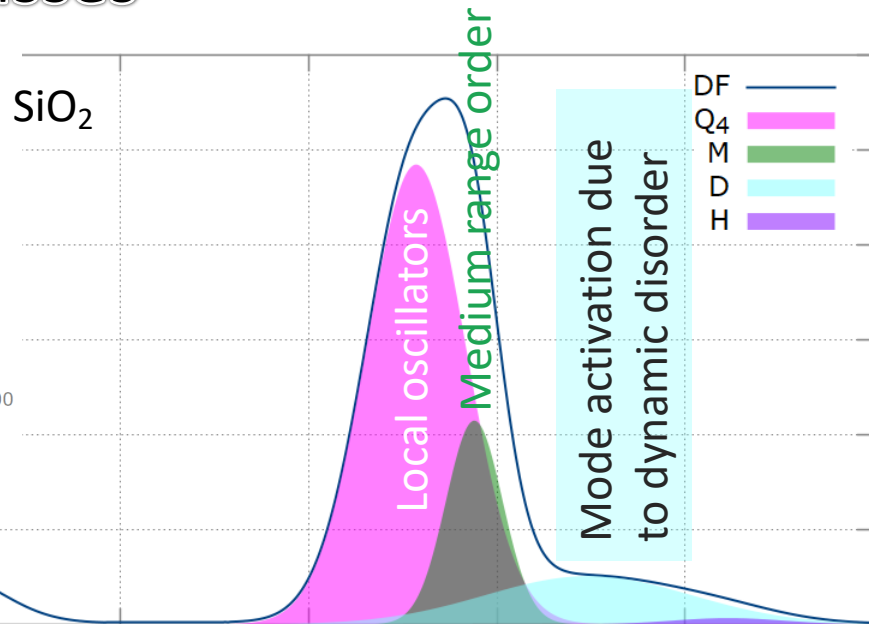
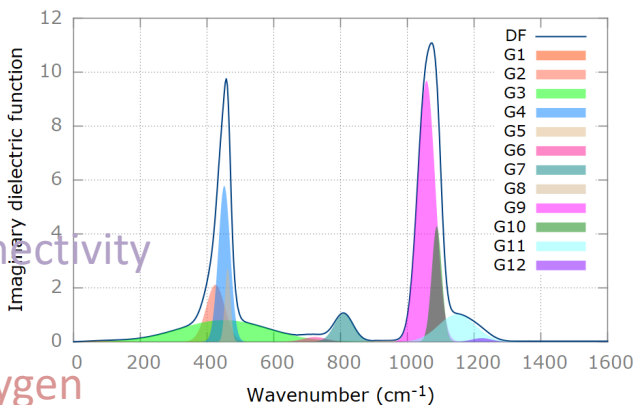


Dynamics of a silica glass versus temperature

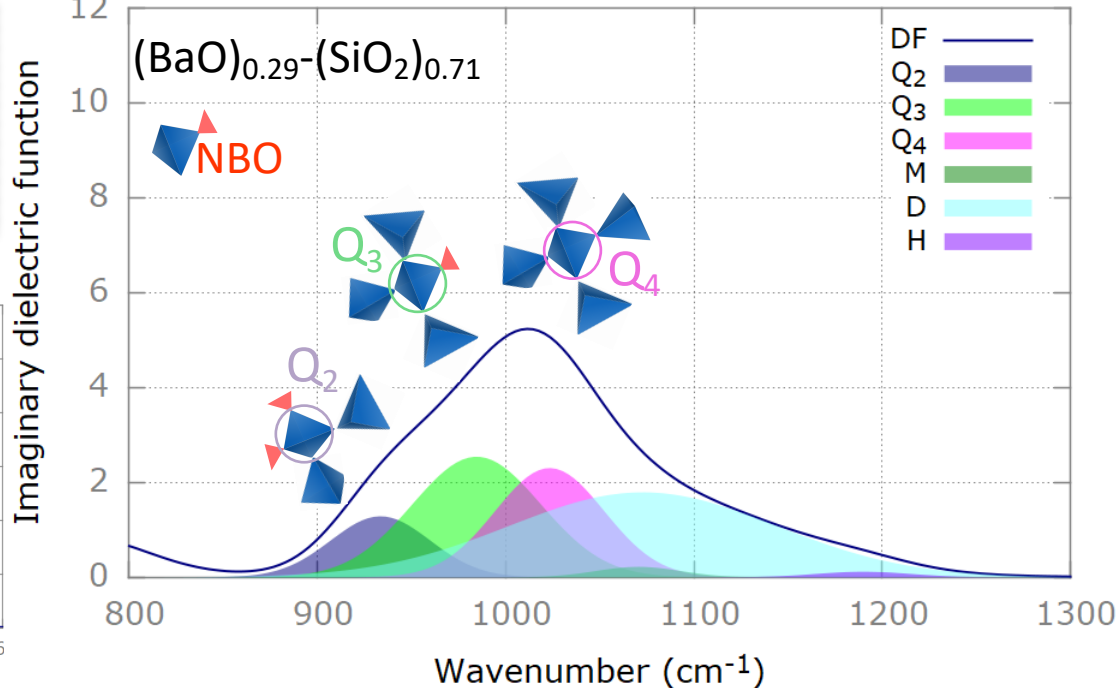
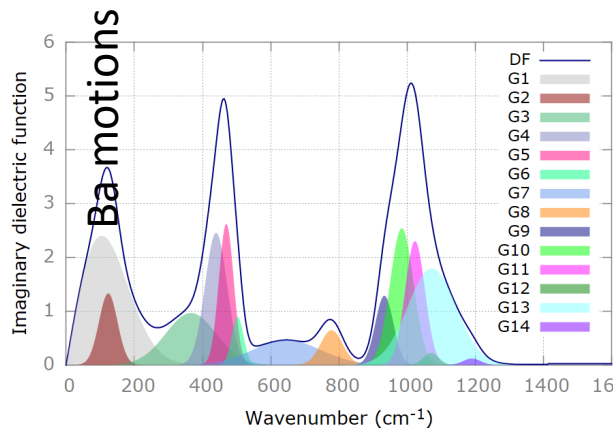


Infrared response of silicate glasses

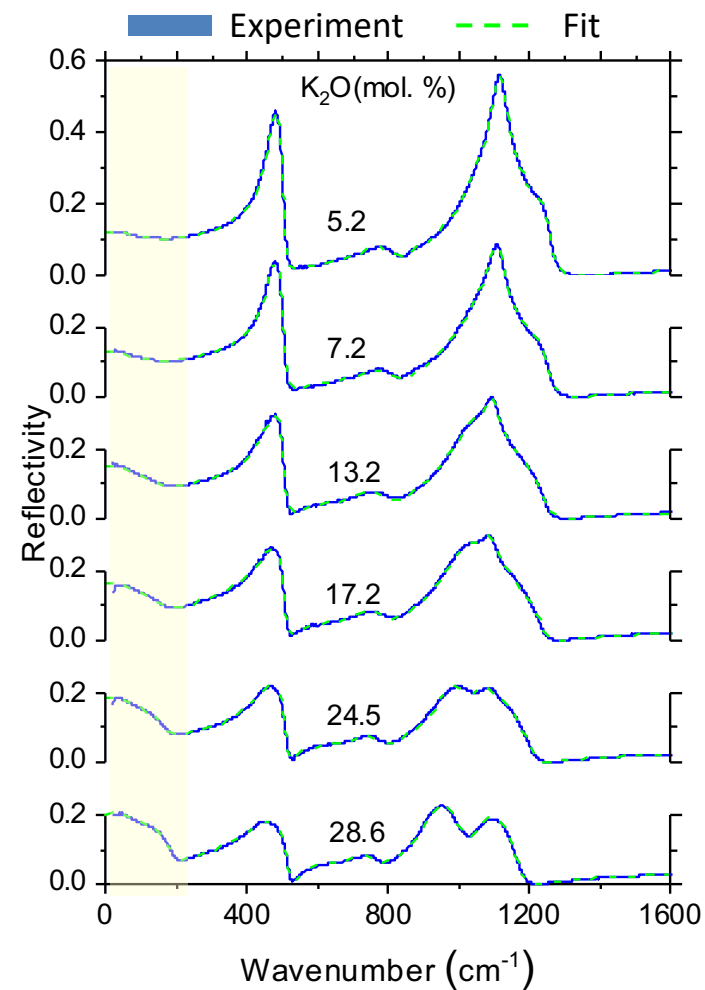
tetrahedra
 stretching
 bridging oxygen
 short range order
 dynamic disorder
 medium range order
 structural disorder
 local oscillators
 modifiers
 network connectivity
 non-bridging oxygen
 oscillators



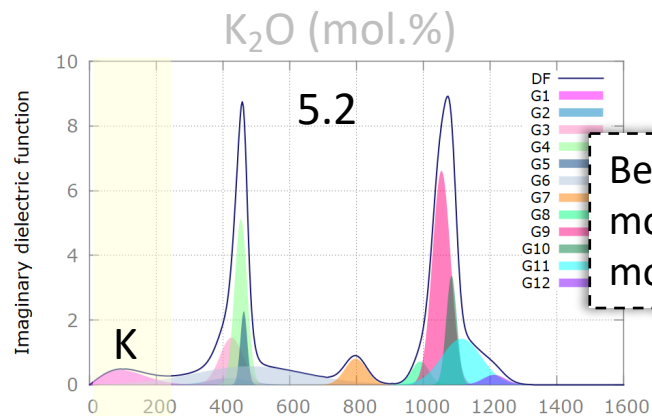
Gaussian components give information on the silicate network dynamics, cation motions, network connectivity, short and medium range order....



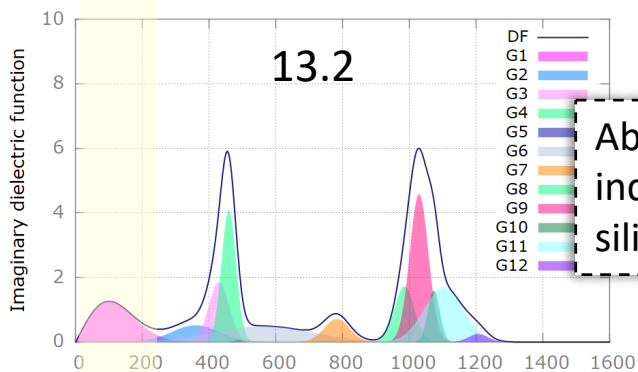
K₂O - SiO₂ glass system



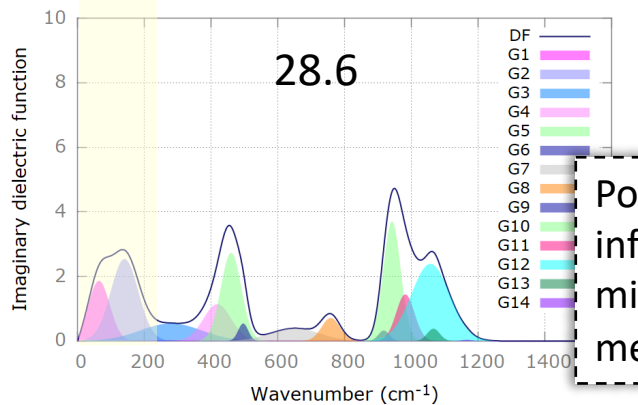
Strong evolution of the reflection spectrum with the increase of the K₂O content.



Below 200 cm⁻¹, vibrational modes are due to potassium motions.



Above 200 cm⁻¹, modes are induced by vibrations of the silicate network.

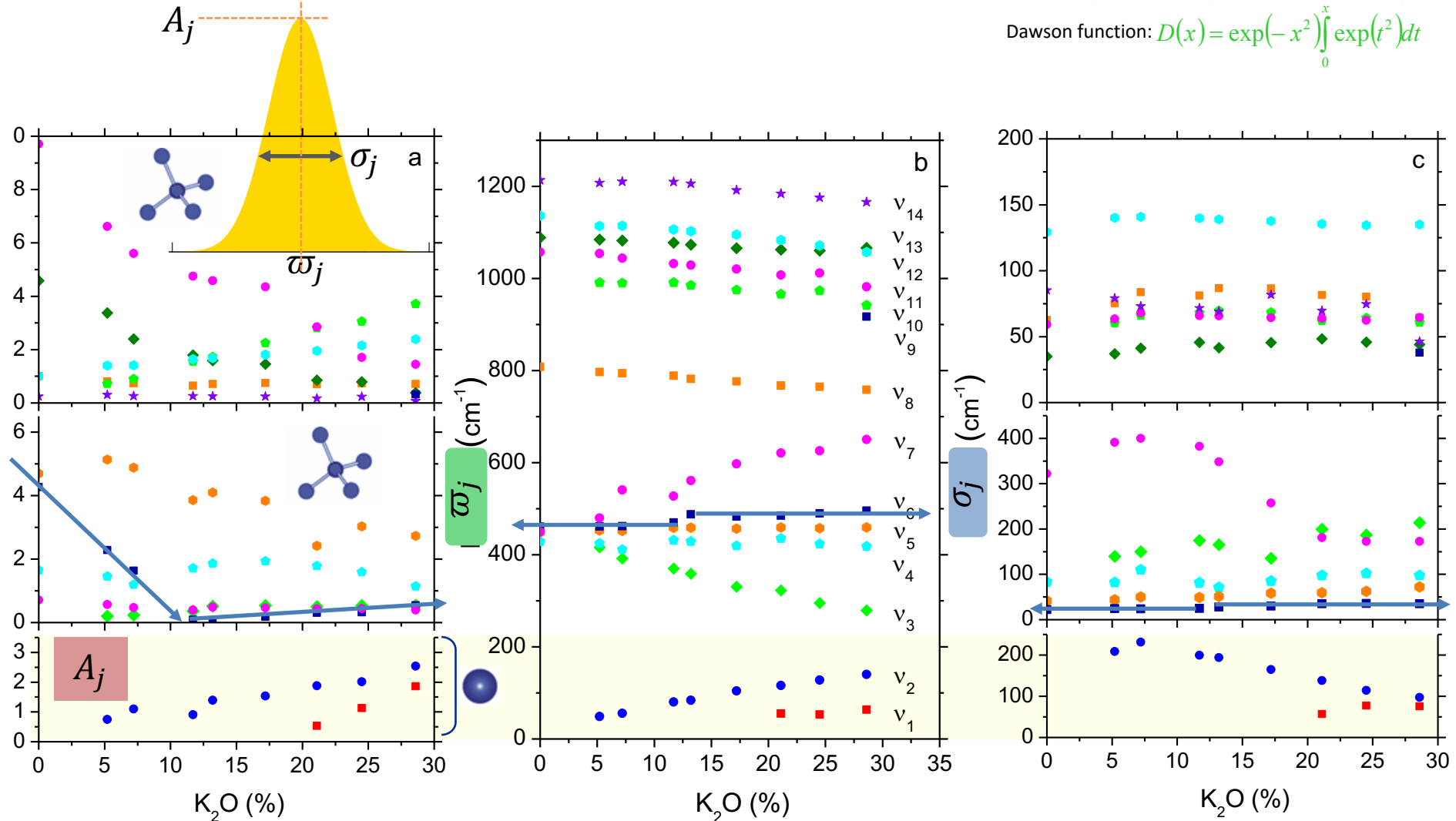


Possibility of extracting information on the glass microstructure at short and medium distances.

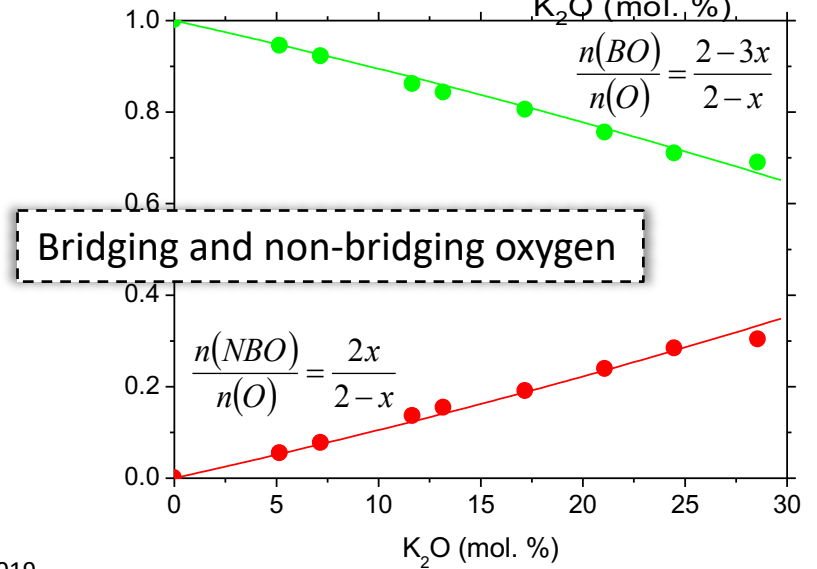
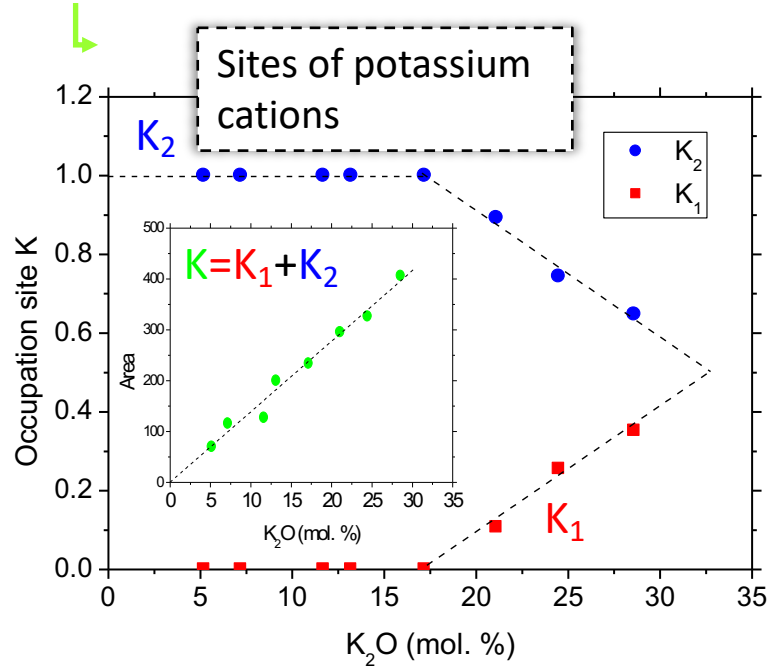
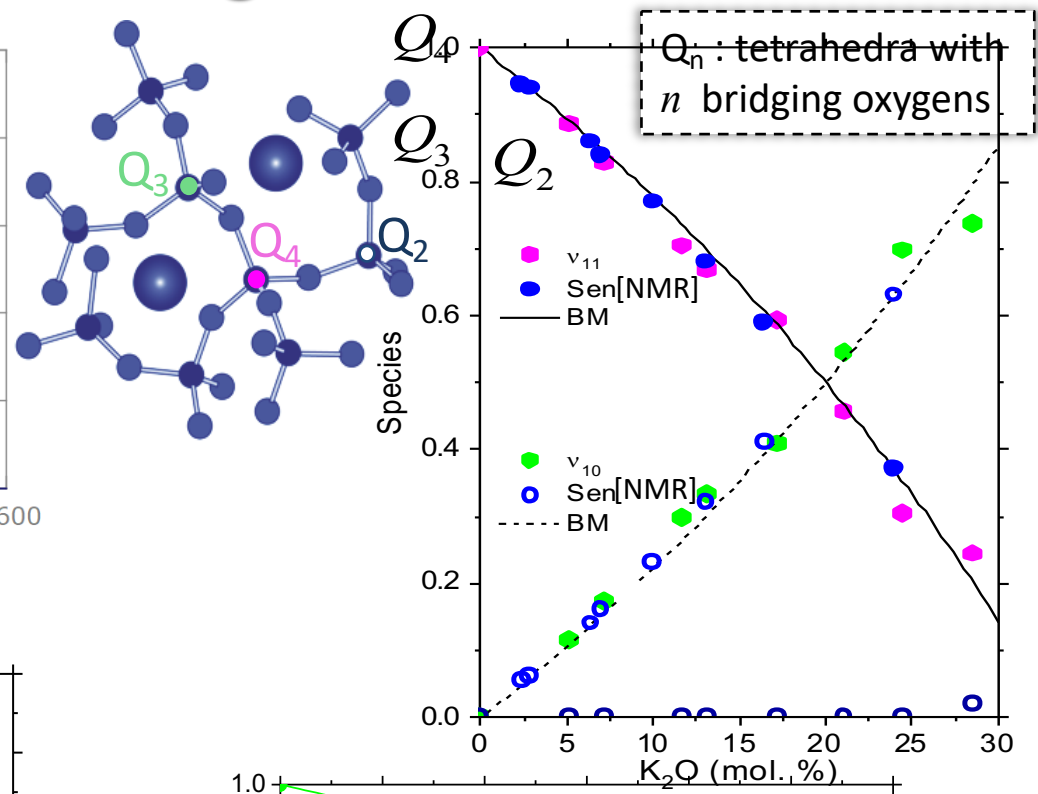
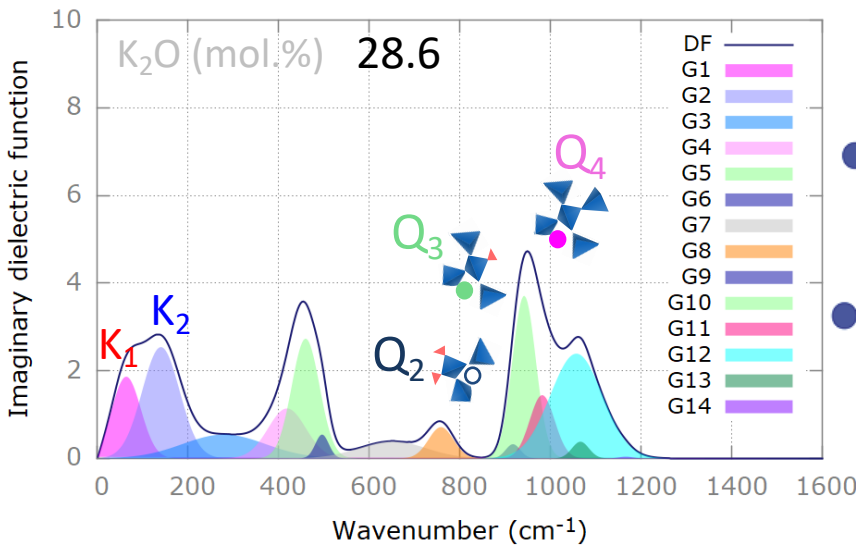
K₂O - SiO₂ glass system

$$\varepsilon(\omega) = \varepsilon_{\infty} + \sum_j \frac{2A_j}{\sqrt{\pi}} \left[D\left(2\sqrt{\ln 2} \frac{\omega + \omega_j}{\sigma_j}\right) - D\left(2\sqrt{\ln 2} \frac{\omega - \omega_j}{\sigma_j}\right) \right] + i A_j \left[\exp\left(-4\ln 2 \left(\frac{\omega - \omega_j}{\sigma_j}\right)^2\right) - \exp\left(-4\ln 2 \left(\frac{\omega + \omega_j}{\sigma_j}\right)^2\right) \right]$$

Dawson function: $D(x) = \exp(-x^2) \int_0^x \exp(t^2) dt$

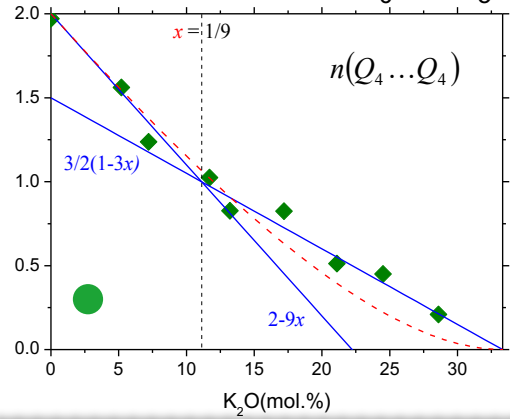
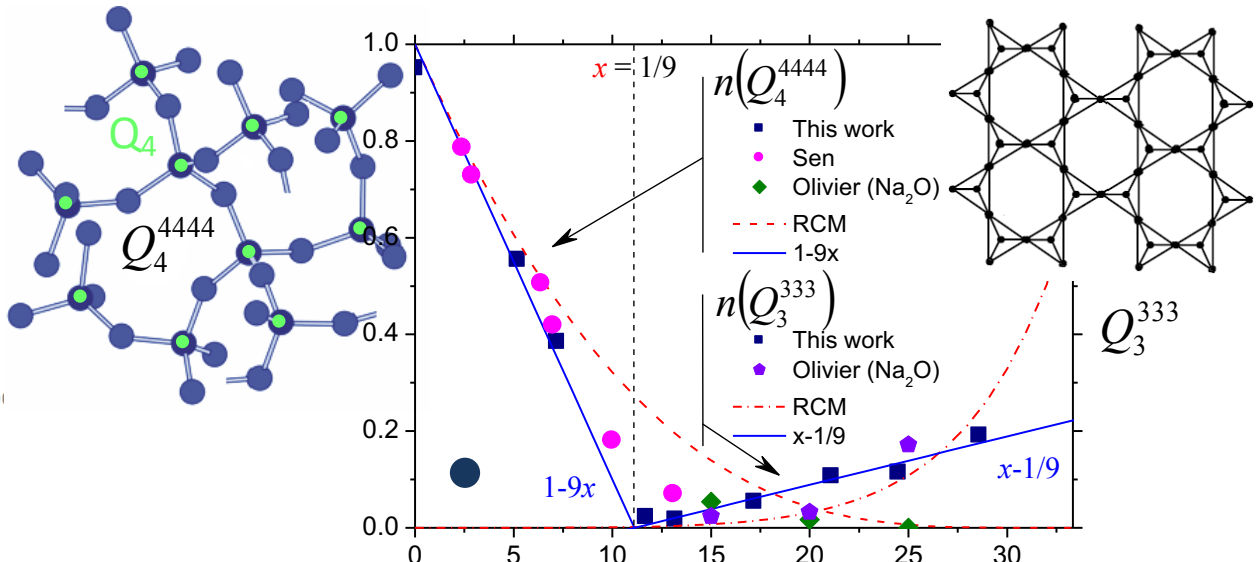
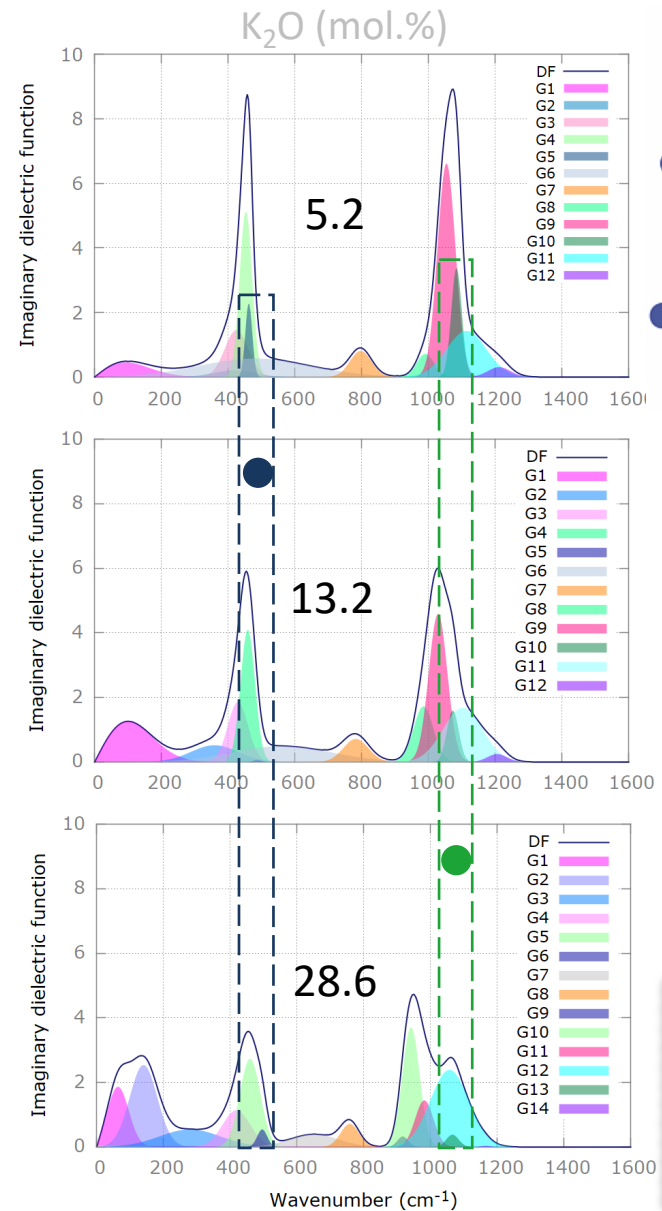


K₂O - SiO₂ glass system : short range order

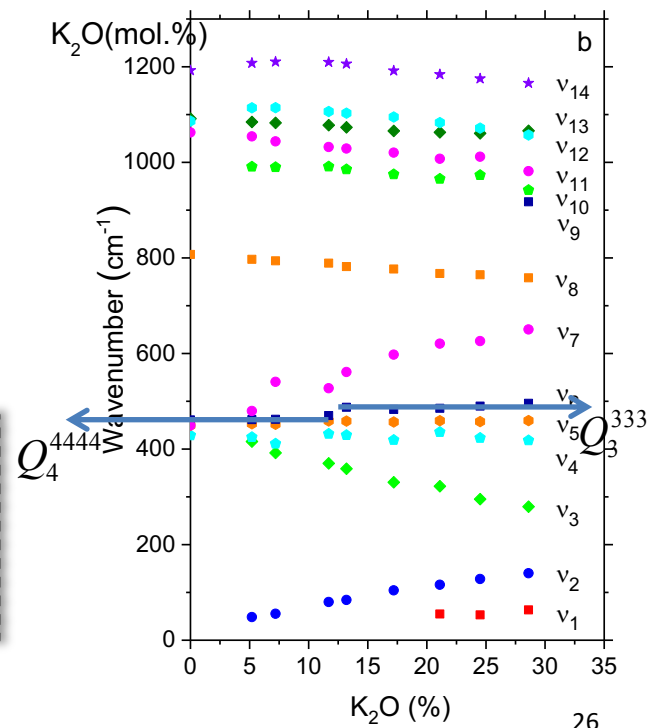


[NMR] Sen S, Youngman R E 2003 *J. Non-Cryst. Solids* 331 100
 [BM] Binary model

K₂O - SiO₂ glass system : medium range order



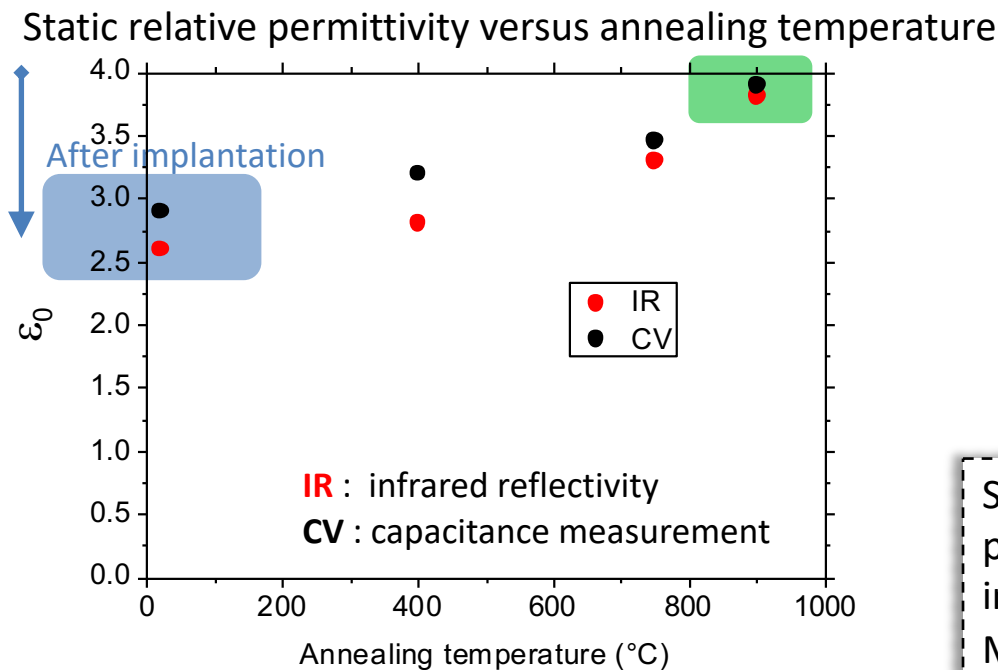
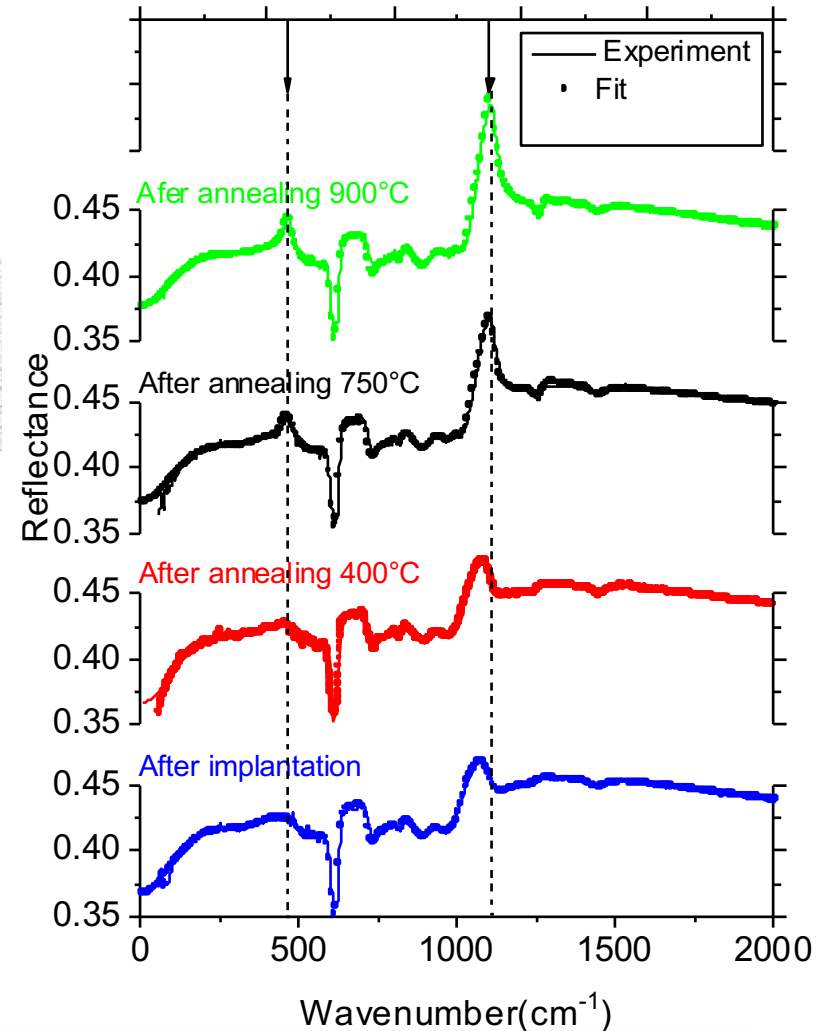
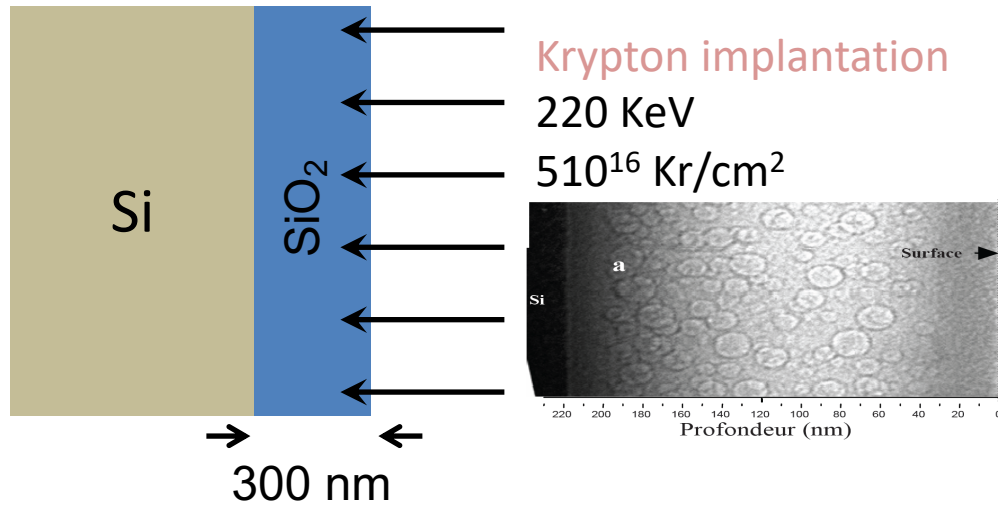
Random Connectivity Model does not explain the glass structure. Depolymerization follows a specific path.



[NMR] Sen S, Youngman R E 2003 *J. Non-Cryst. Solids* 331 100

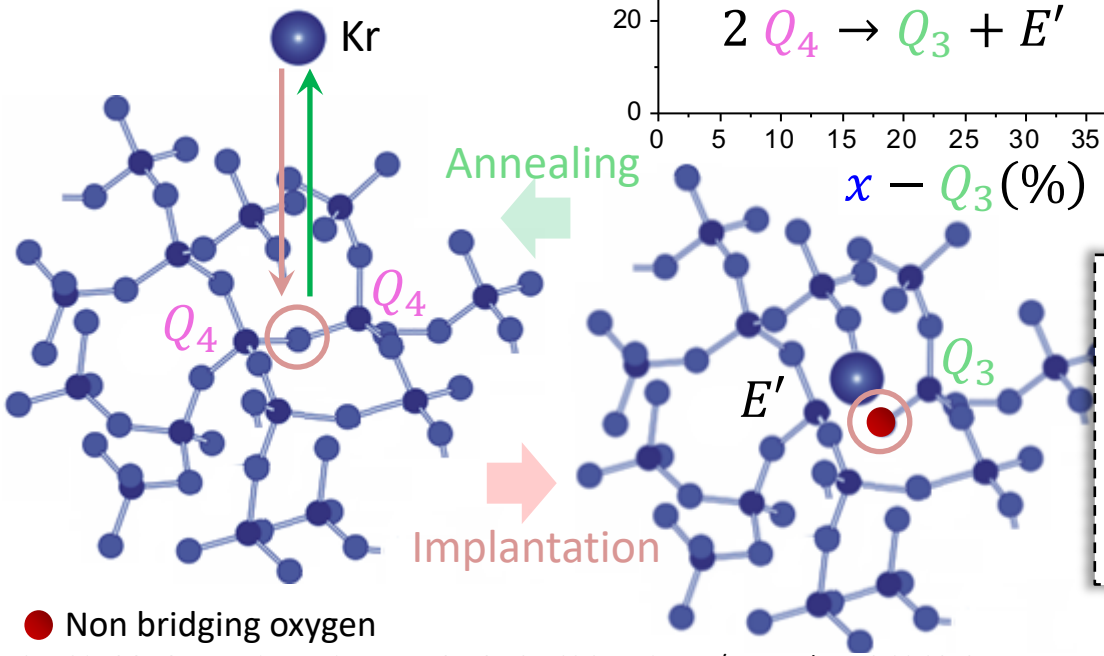
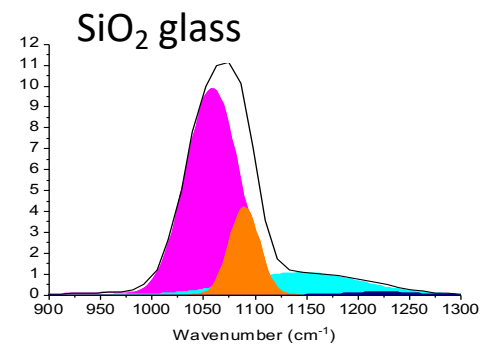
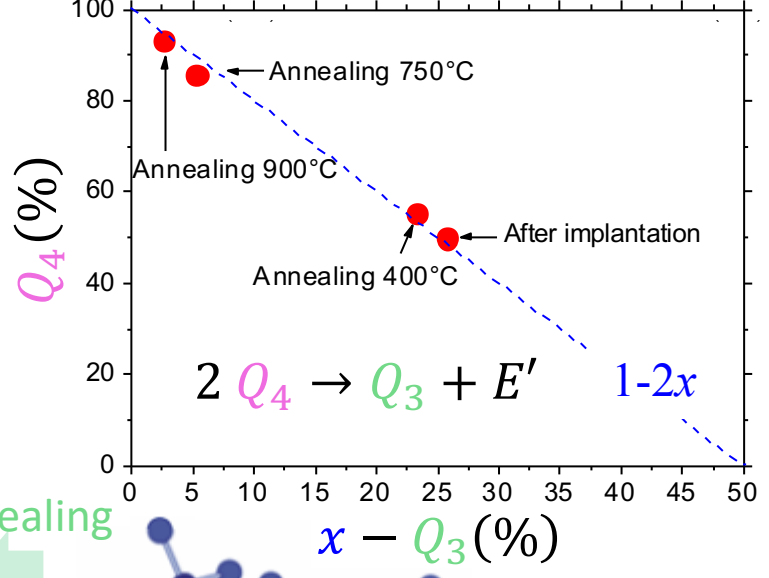
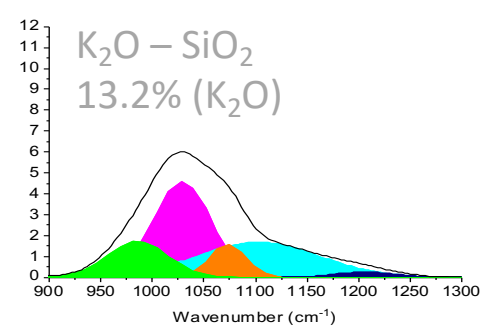
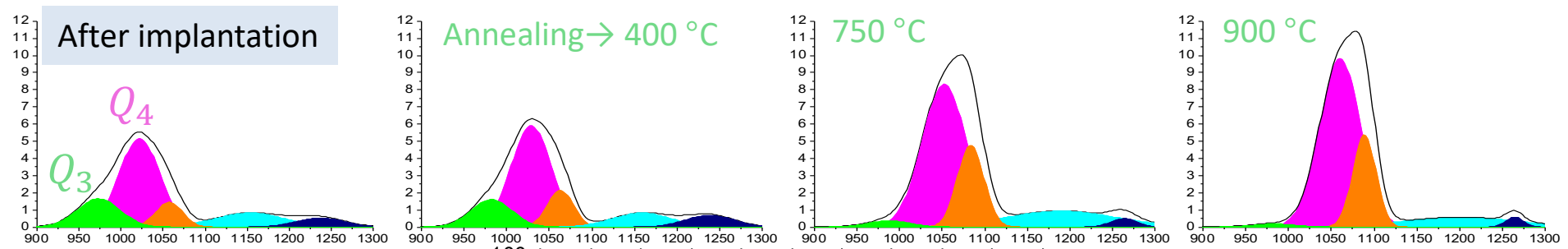
[NMR] Olivier L, Yuan X, Cormack A N, Jäger C 2001 *J. Non-Cryst. Solids* 293-295 53

SiO₂ thin film implanted with Krypton



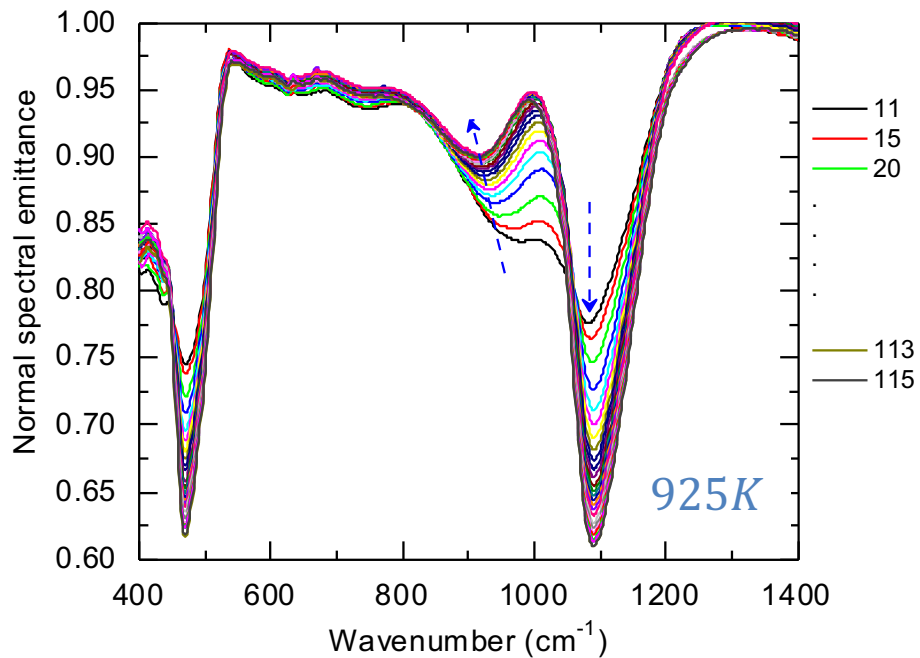
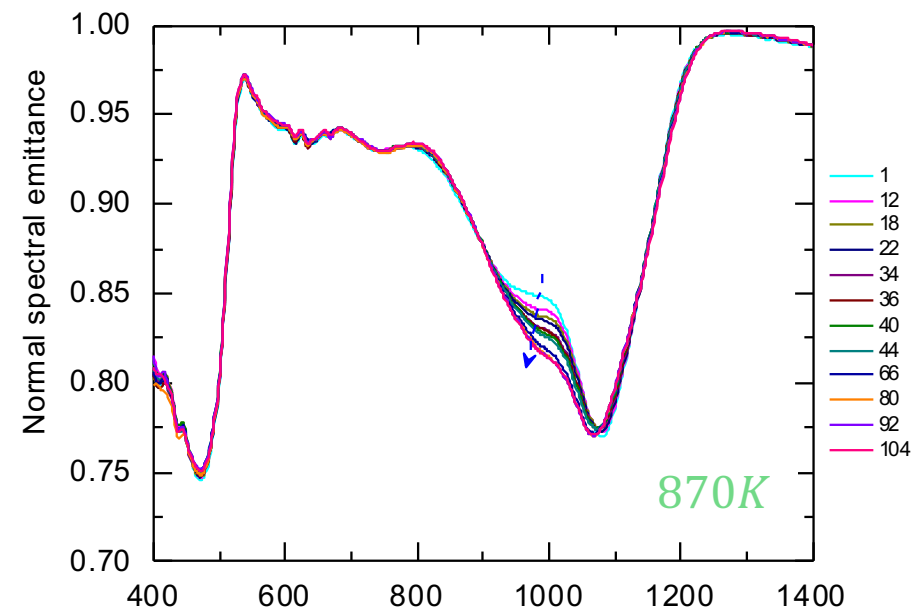
Strong decrease of the static relative permittivity of the SiO₂ thin film after implantation.
 Material healing after annealing at 900 °C

SiO₂ thin film implanted with Krypton



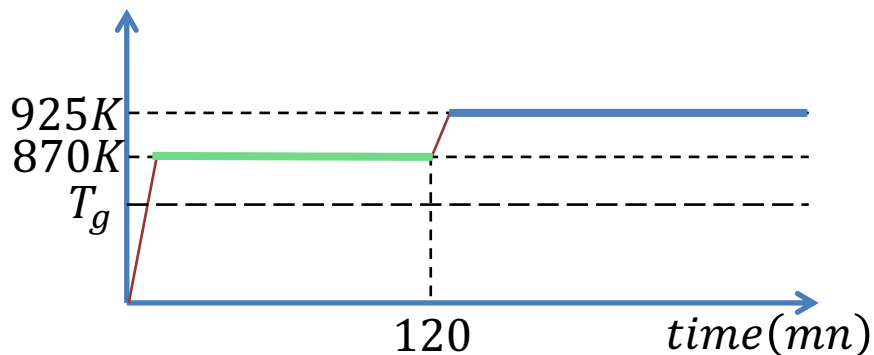
Implantation mechanism
 Damage of the silicate network by creating E' centers and Q_3 structural units.
 Loss of 50% of the Q_4 structural units inducing a diminution of the vibrational contribution to the static permittivity.

Structural relaxation of a silicate glass



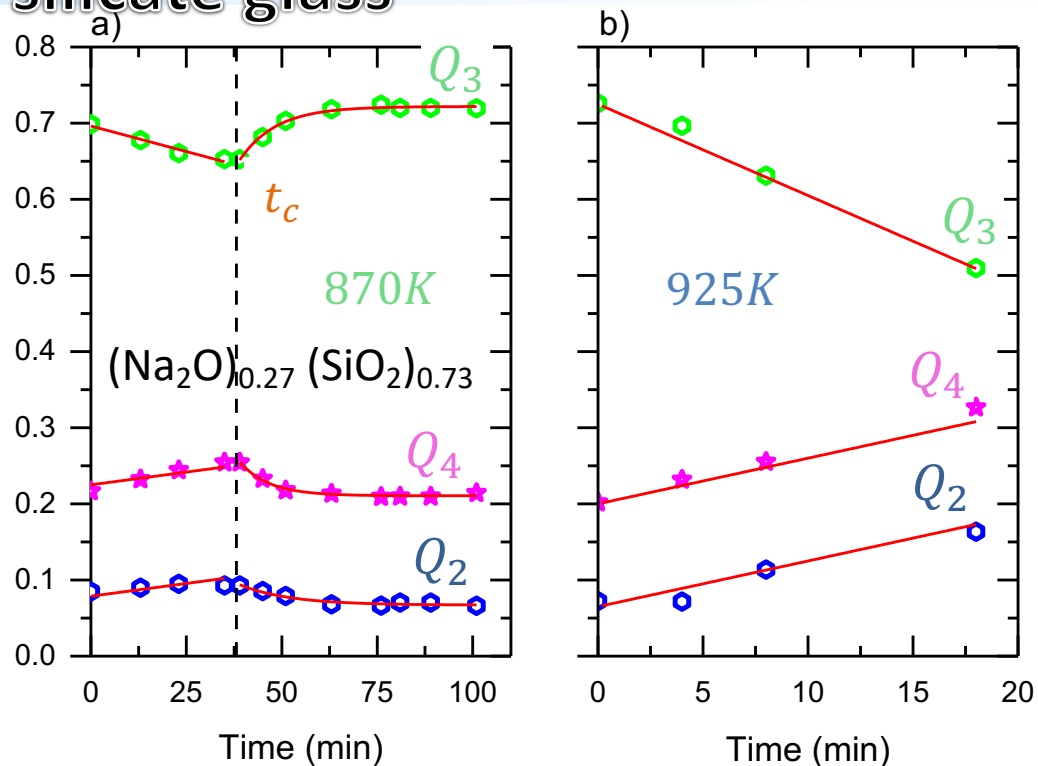
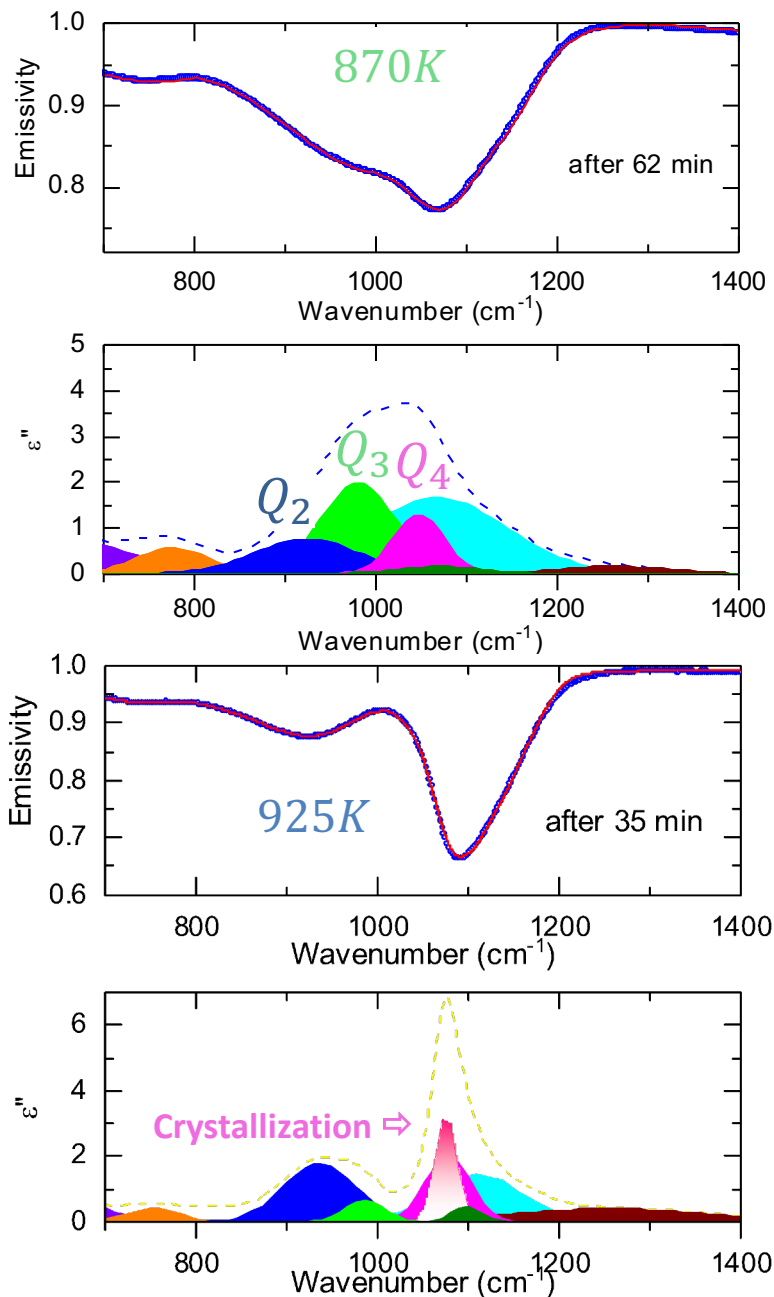
$(\text{Na}_2\text{O})_{0.27} (\text{SiO}_2)_{0.73}$ silicate glass

Thermal heat treatment

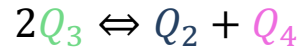


Glass transition temperature (T_g): $\cong 730\text{K}$
Continuous acquisition of spectra during annealing at 870 K and 925K

Structural relaxation of a silicate glass



Annealing at 870 K does not lead to crystallization of the glass.



First step, small shift of the chemical equilibrium to the right.

After t_c , structural relaxation ($\tau \cong 10 \text{ mn}$) and shift to the left of the chemical equilibrium.

$$Q_n(t) = c_n \exp\left(-\frac{t-t_c}{\tau}\right) + d_n$$

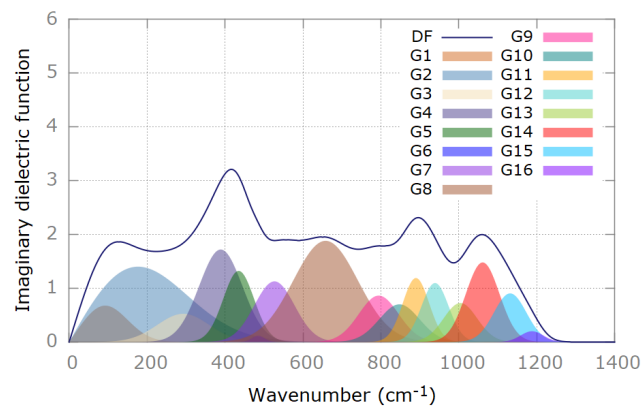
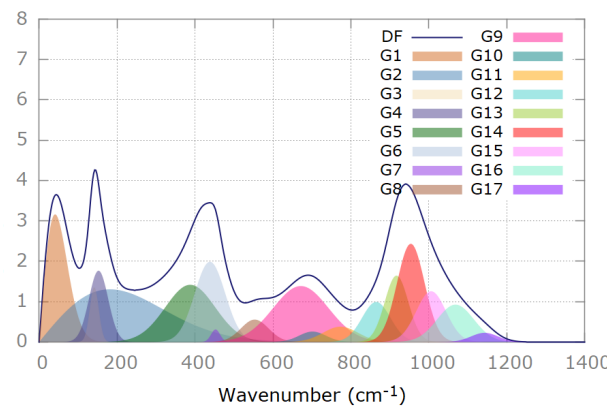
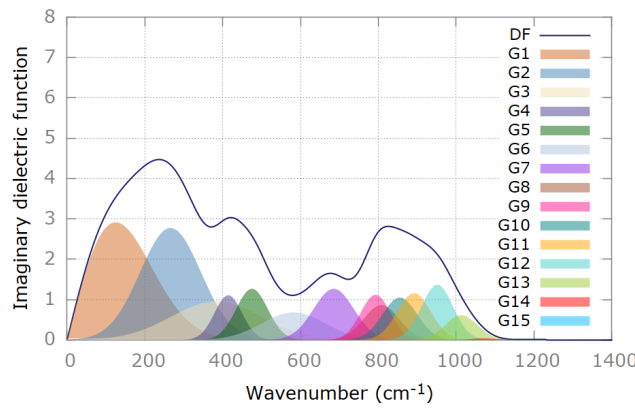
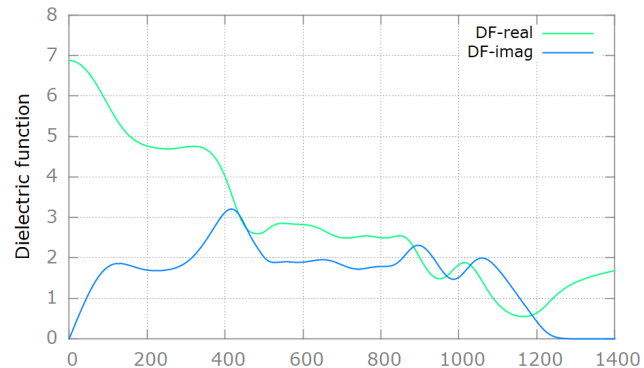
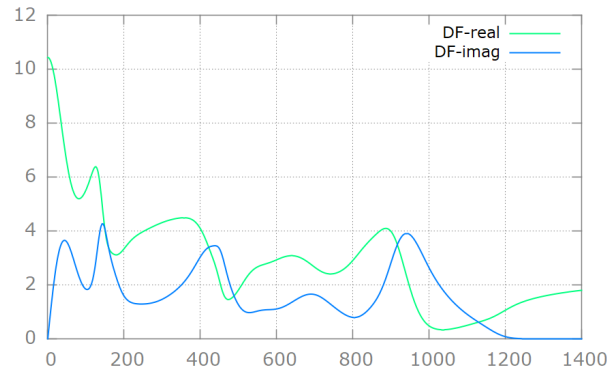
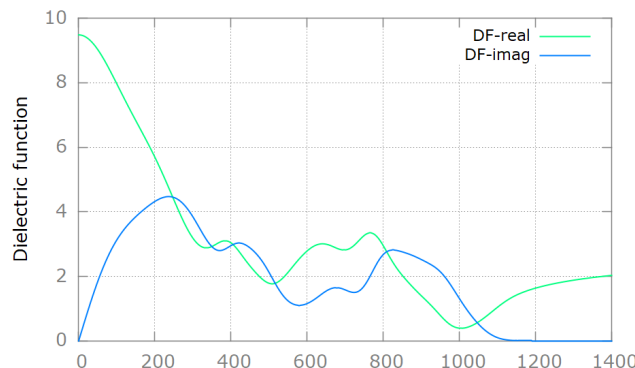
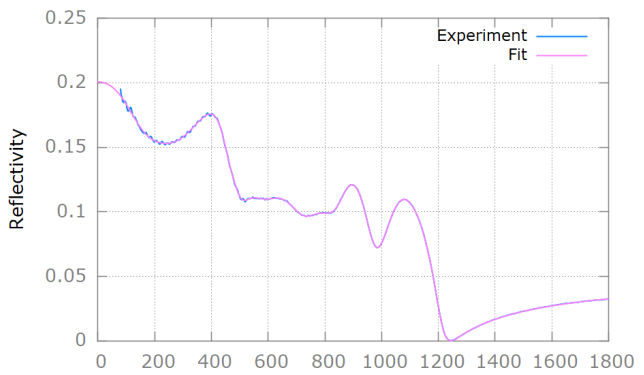
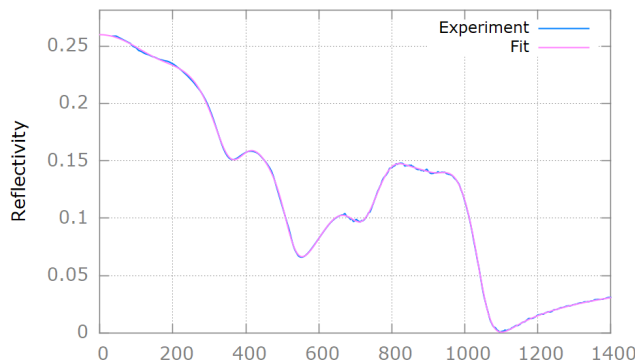
At 925 K crystallization is evidenced after 20 mn.

Infrared response of aluminosilicate glasses

Ca₂Al₂SiO₇ glass

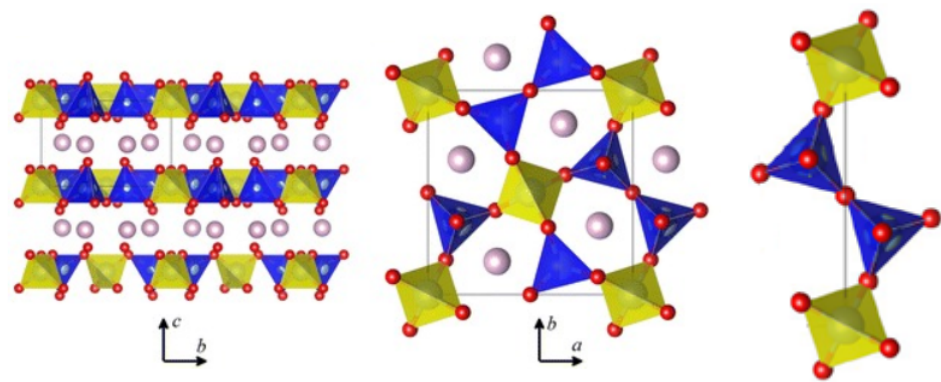
BaAl₂Si₂O₈ glass

ZnAl₂Si₂O₈ glass



Infrared response of aluminosilicate glasses

Crystal structure of gehlenite



Yellow tetrahedra : Wyckoff site 2a labelled T_1 is fully occupied by Al atoms



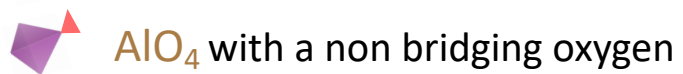
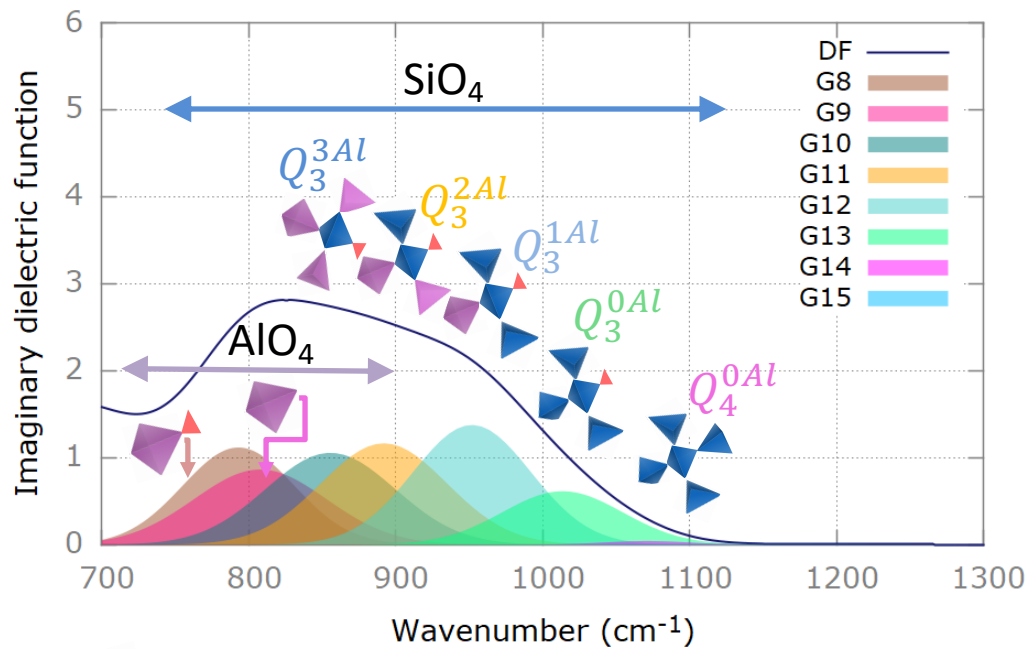
Blue tetrahedra : Wyckoff site 4e, labelled T_2 is filled with a mix of Al (50 %) and Si (50 %) atoms



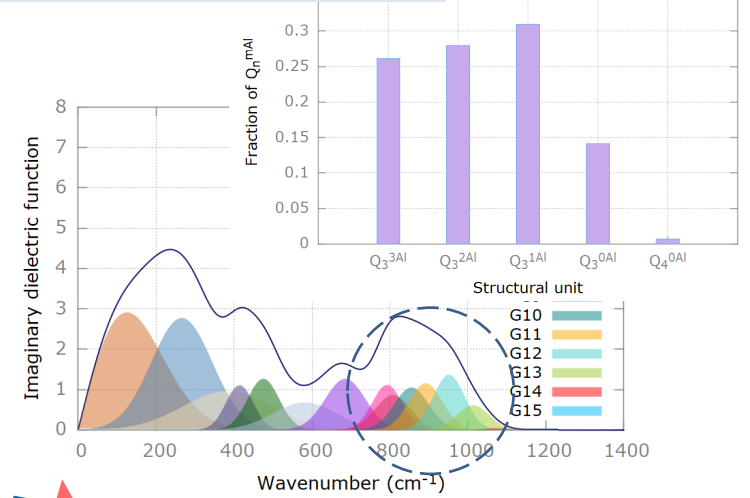
100% Q_3^{3Al}



$Ca_2Al_2SiO_7$ glass



Q_n^{mAl} structural units



SiO_4 with a non bridging oxygen

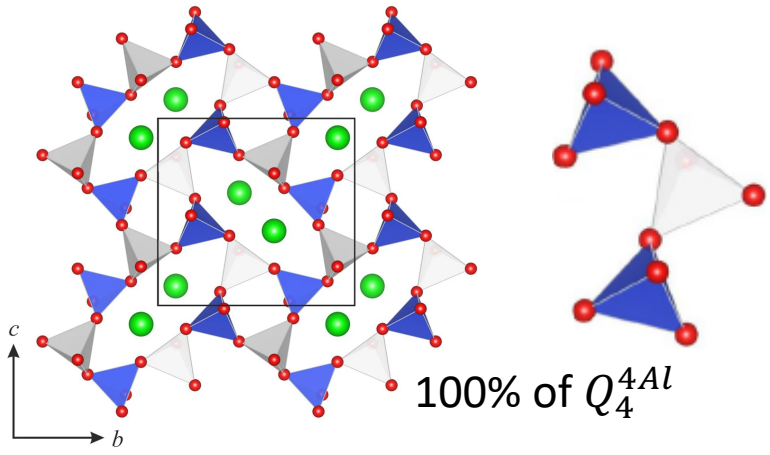
Access to structural information

Q_n^{mAl} structural units

Nature of AlO_4 tetrahedra

Infrared response of aluminosilicate glasses

Crystal structure of $BaAl_2Si_2O_8$ (paracelsian)



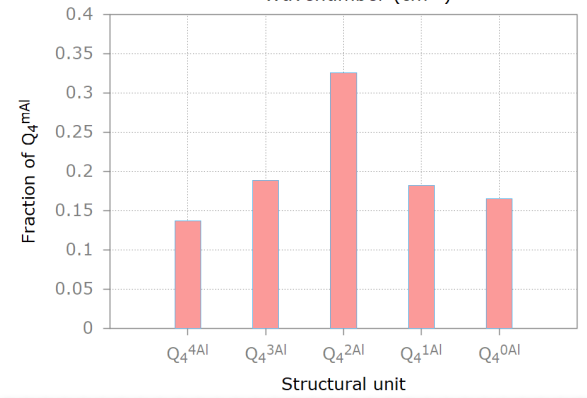
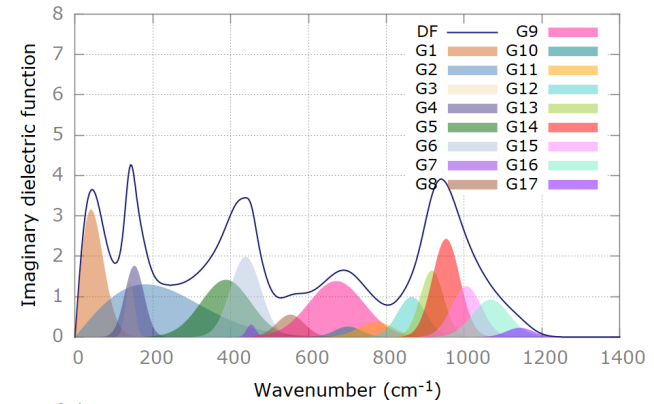
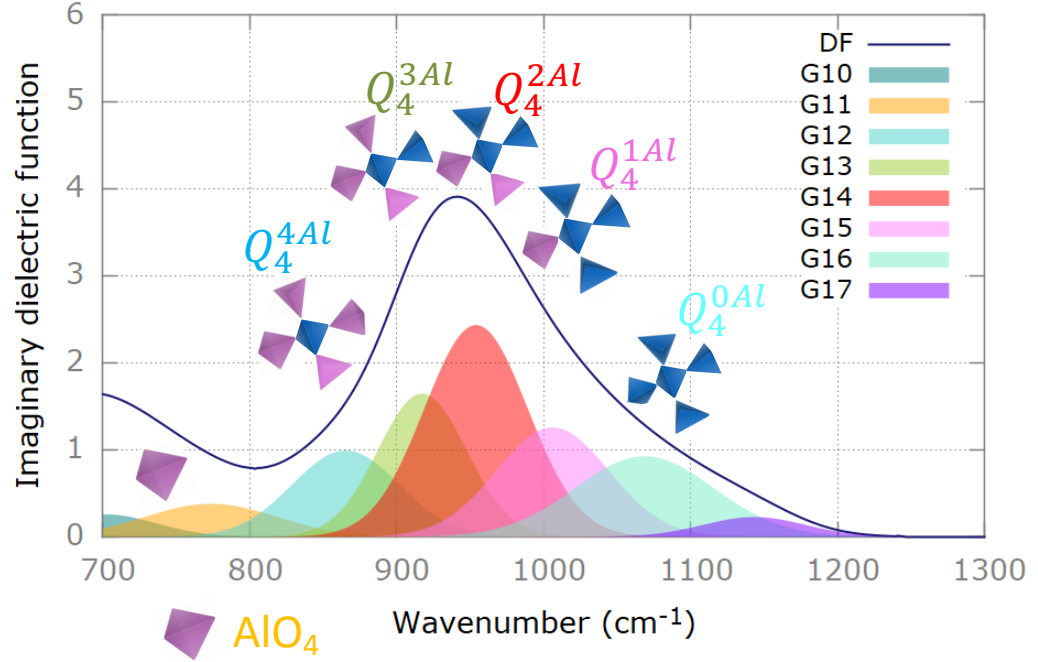
Blue tetrahedra : Al atoms (AlO_4) surrounded by 4 Al atoms.

Gray tetrahedra : Si atoms (SiO_4) surrounded by 4 Al atoms.

100% of Q_4^{4Al}

$BaAl_2Si_2O_8$ glass

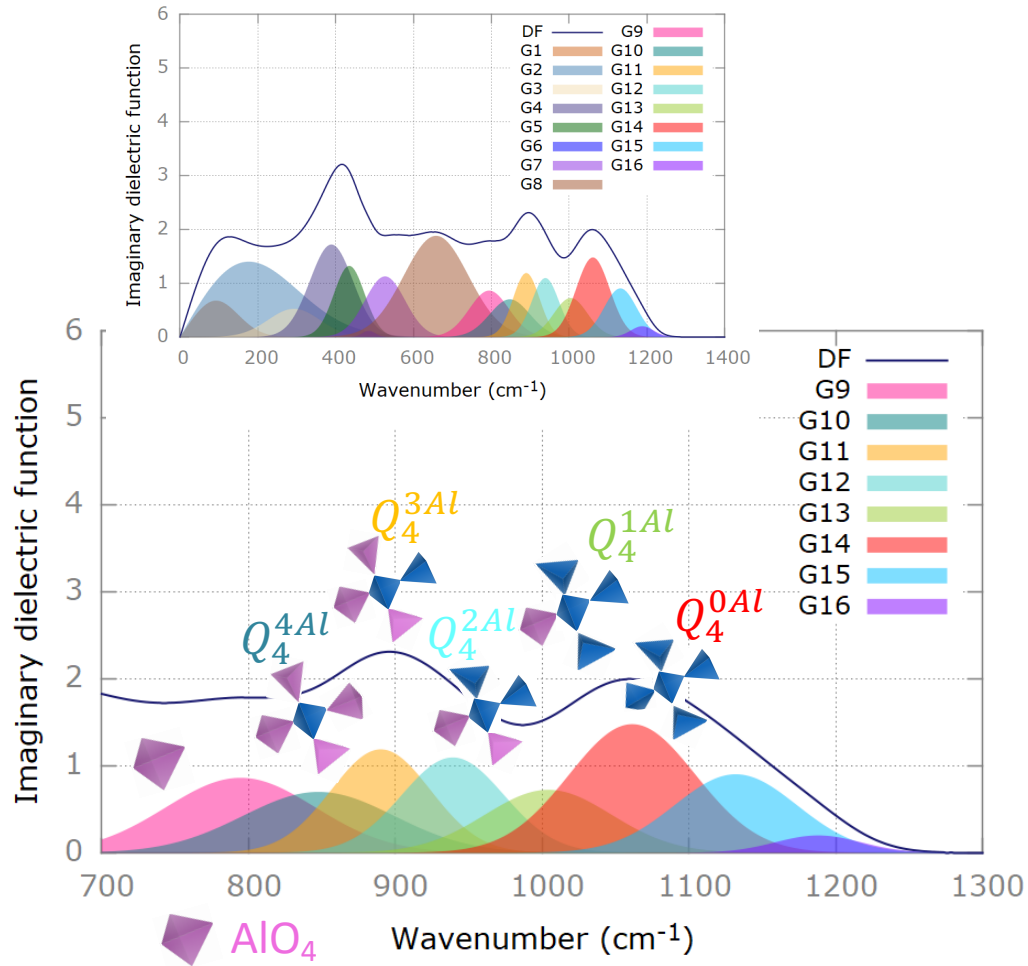
Q_n^{mAl} structural units



Broad distribution of Q_4^{mAl} structural units.
Al-O-Al bonds

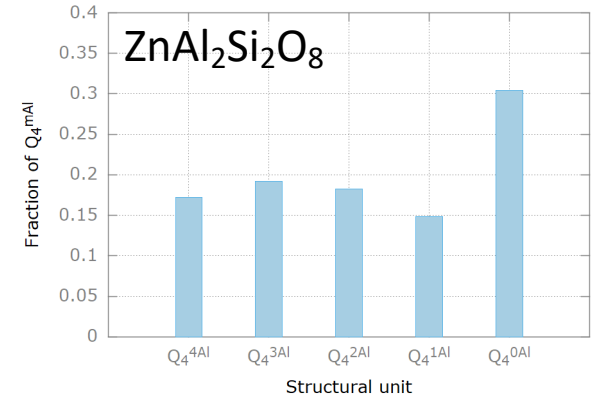
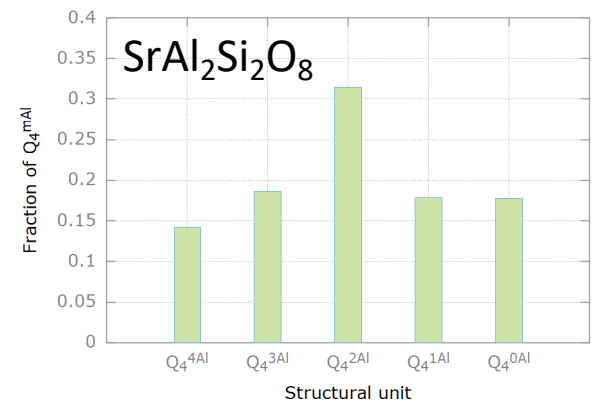
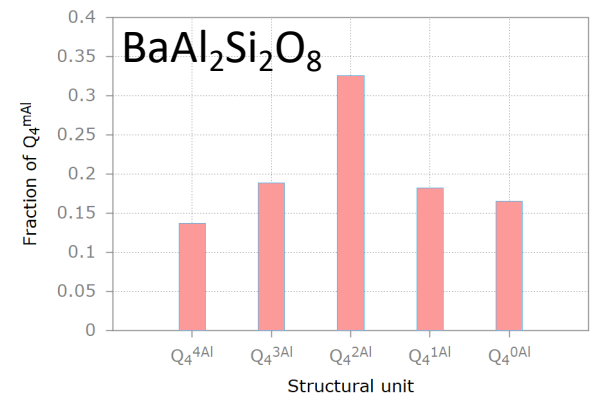
Infrared response of aluminosilicate glasses

ZnAl₂Si₂O₈ glass

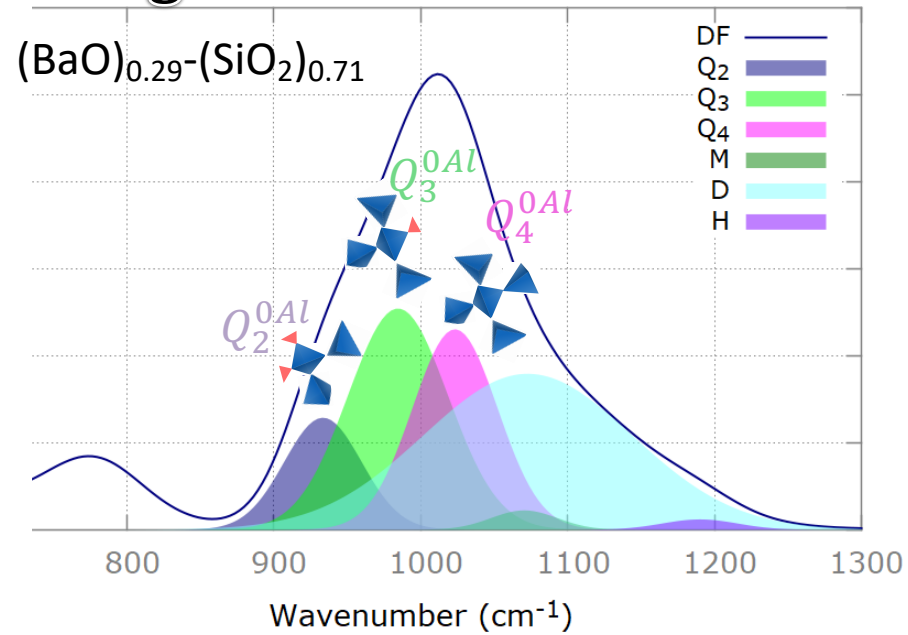
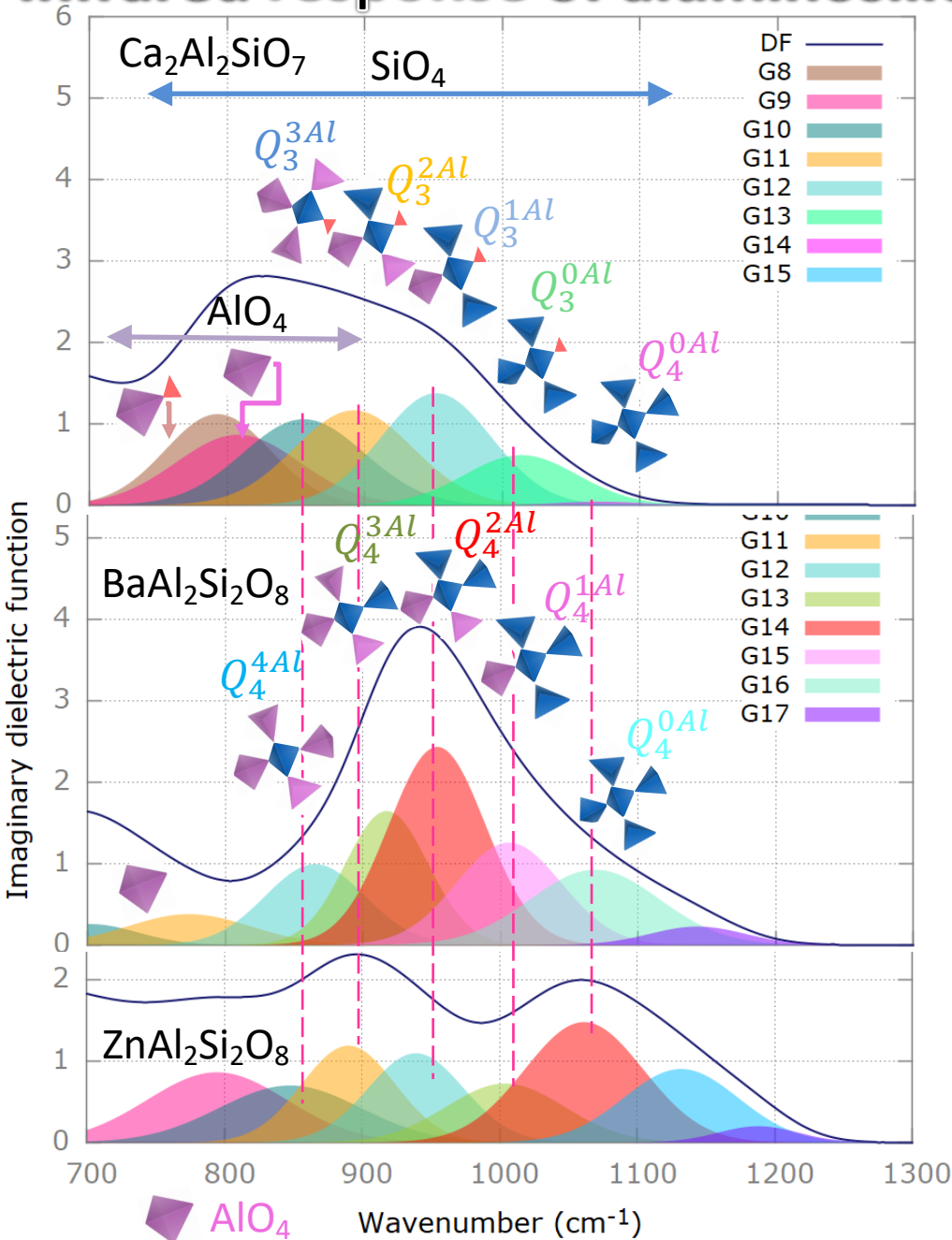


Asymmetric distribution of Q_4^{mAl} structural units for ZnAl₂Si₂O₈.

Q_n^{mAl} structural units



Infrared response of aluminosilicate glasses

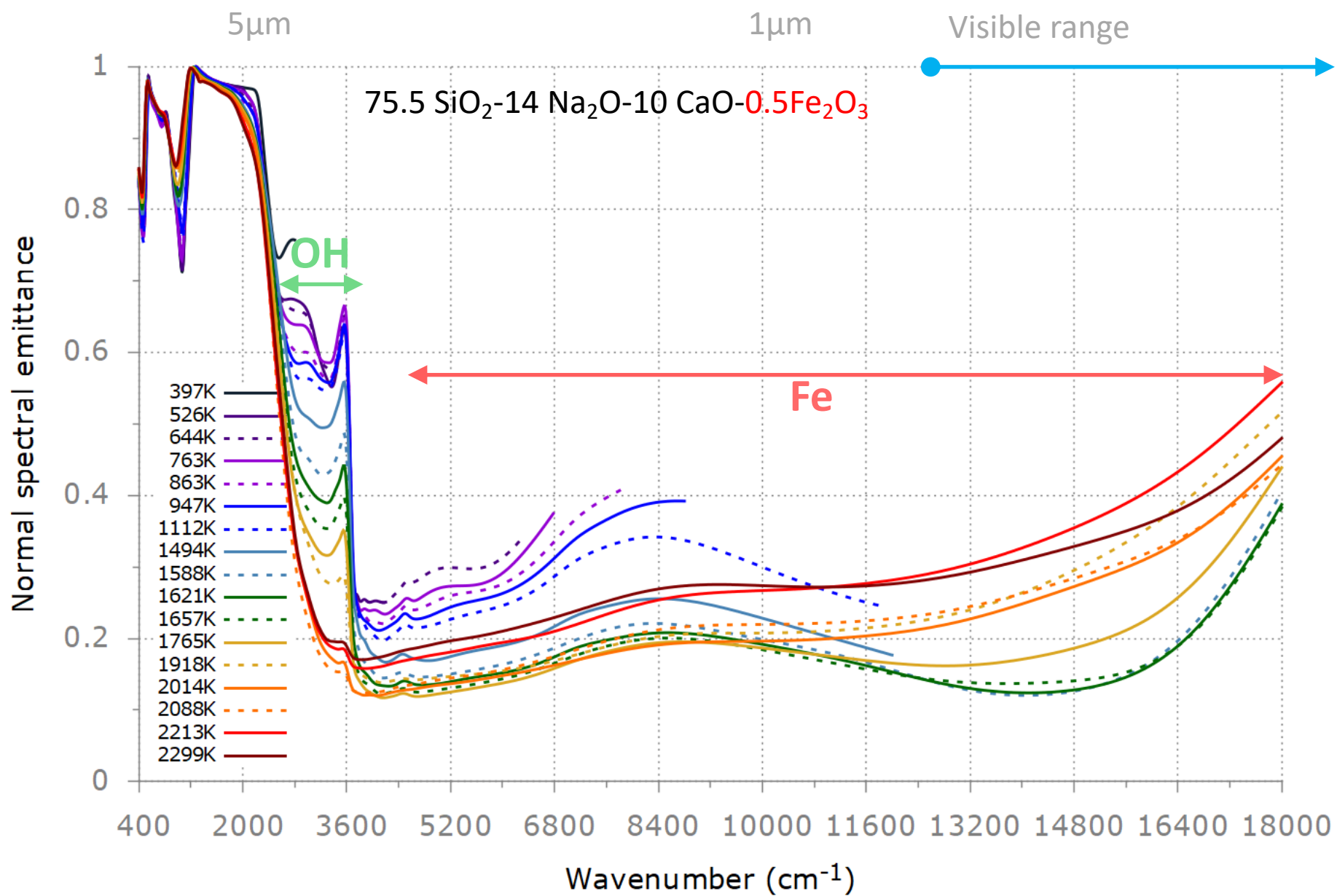


Q_n^{mAl} structural units

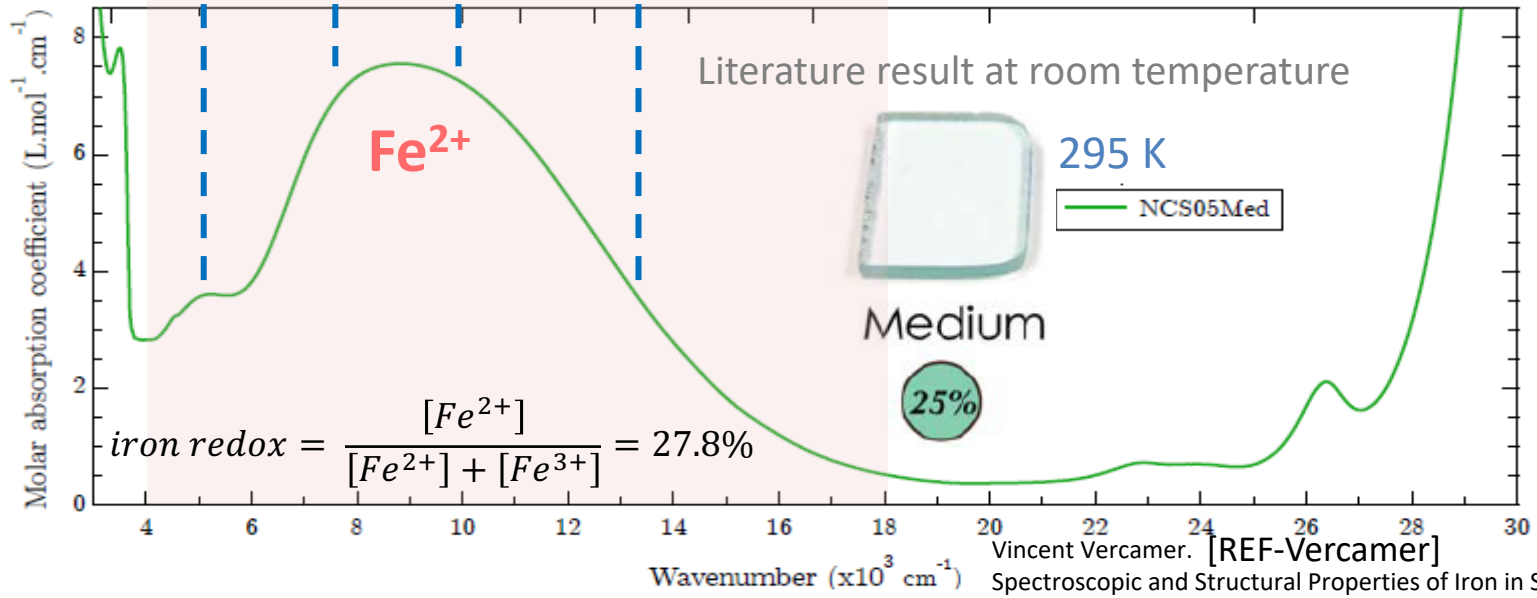
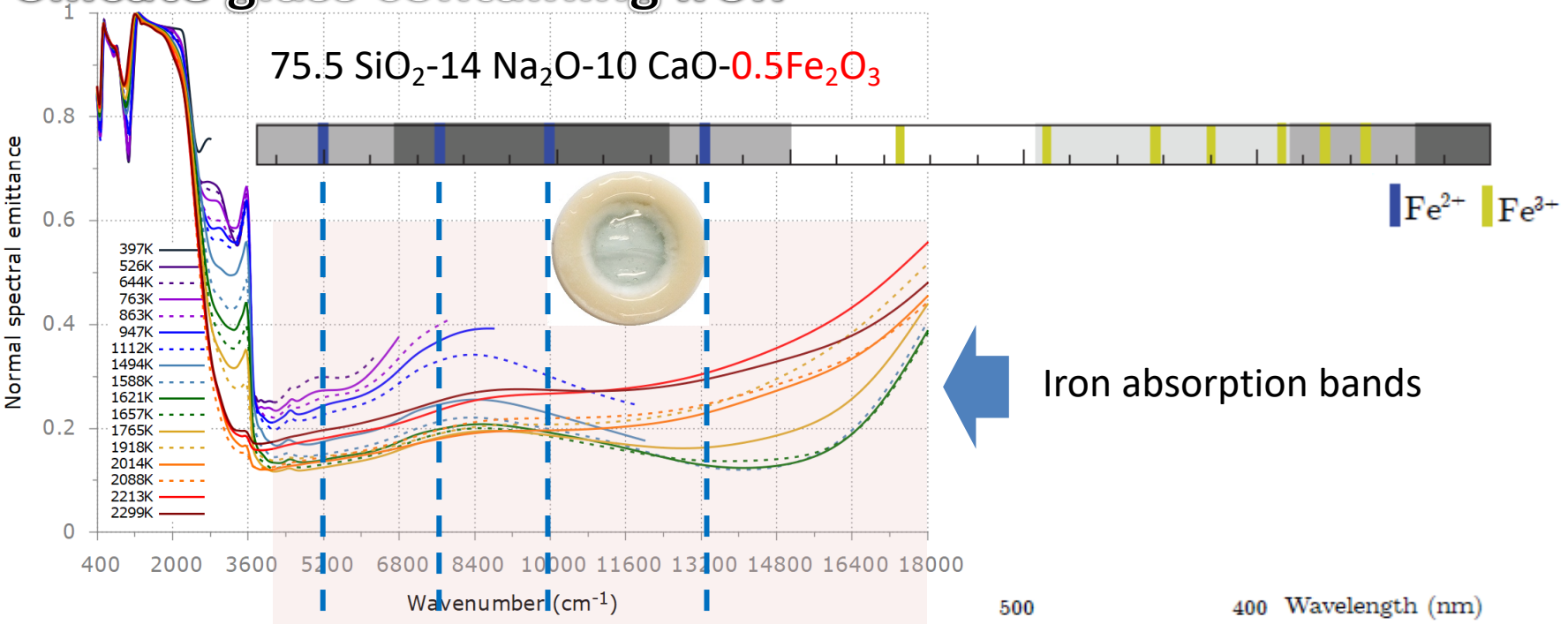
Absorption band position (cm⁻¹)

≈ 860	≈ 900	≈ 950	≈ 1010	≈ 1060
Q_4^{4Al}	Q_4^{3Al}	Q_4^{2Al}	Q_4^{1Al}	Q_4^{0Al}
Q_3^{3Al}	Q_3^{2Al}	Q_3^{1Al}	Q_3^{0Al}	
		Q_2^{0Al}		

Silicate glass containing iron



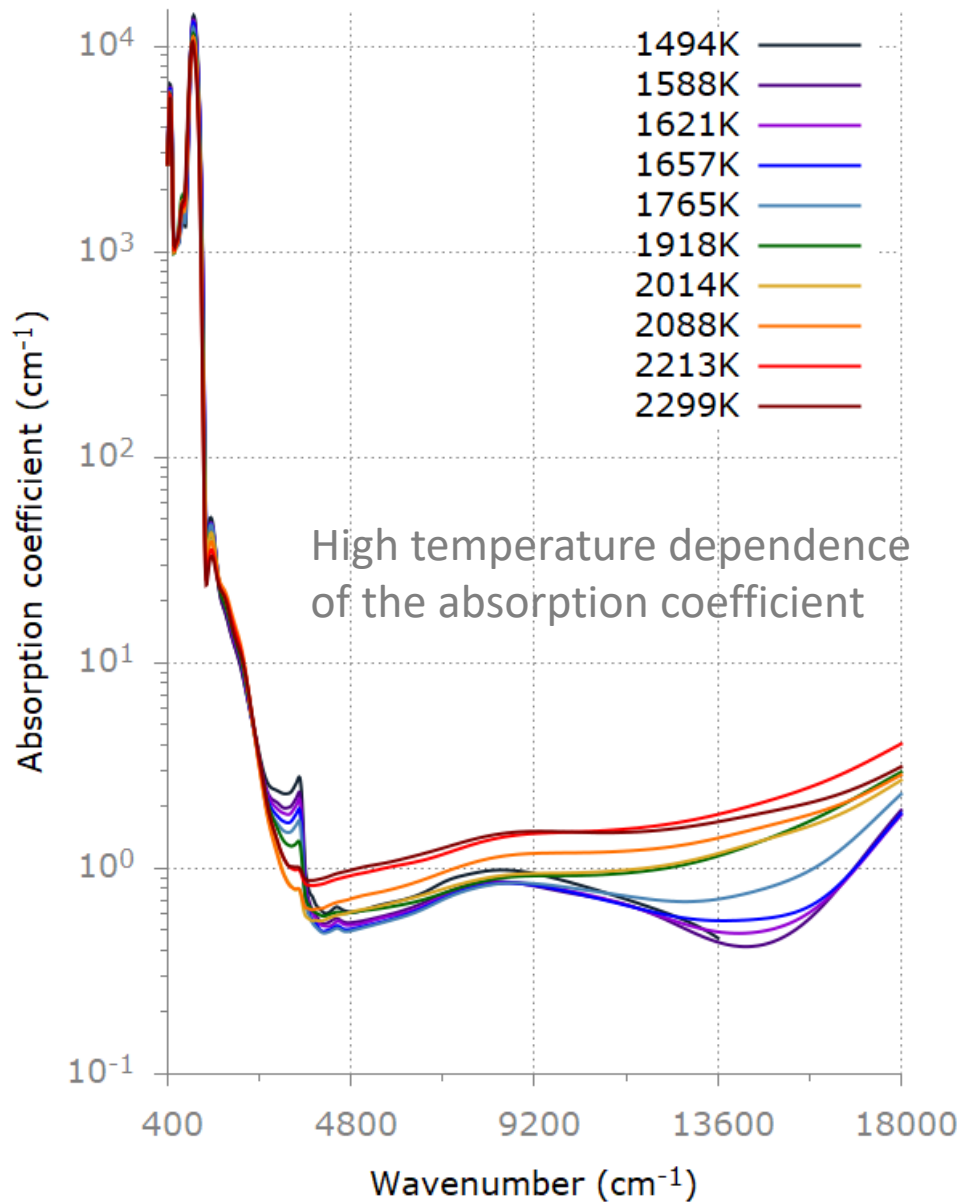
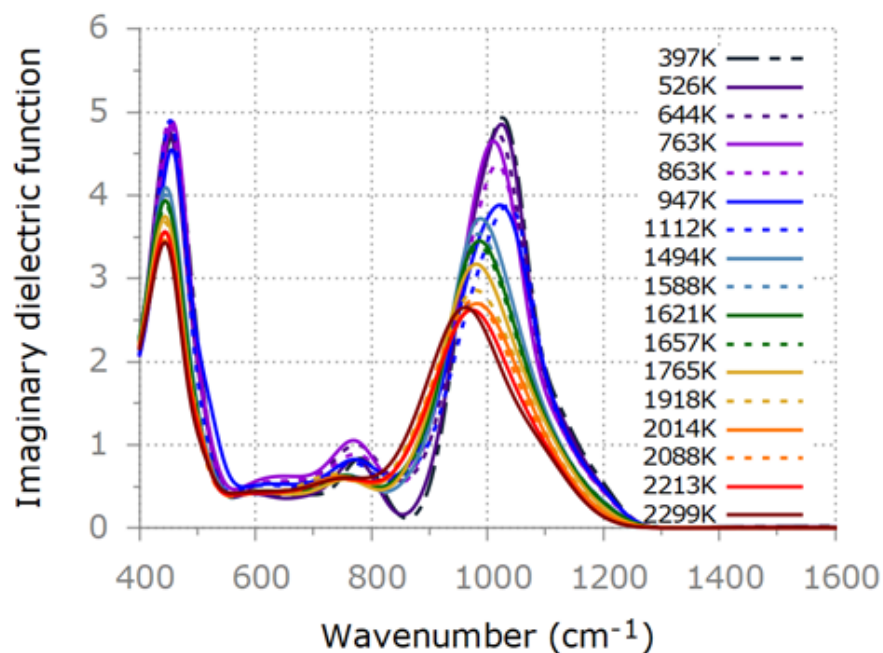
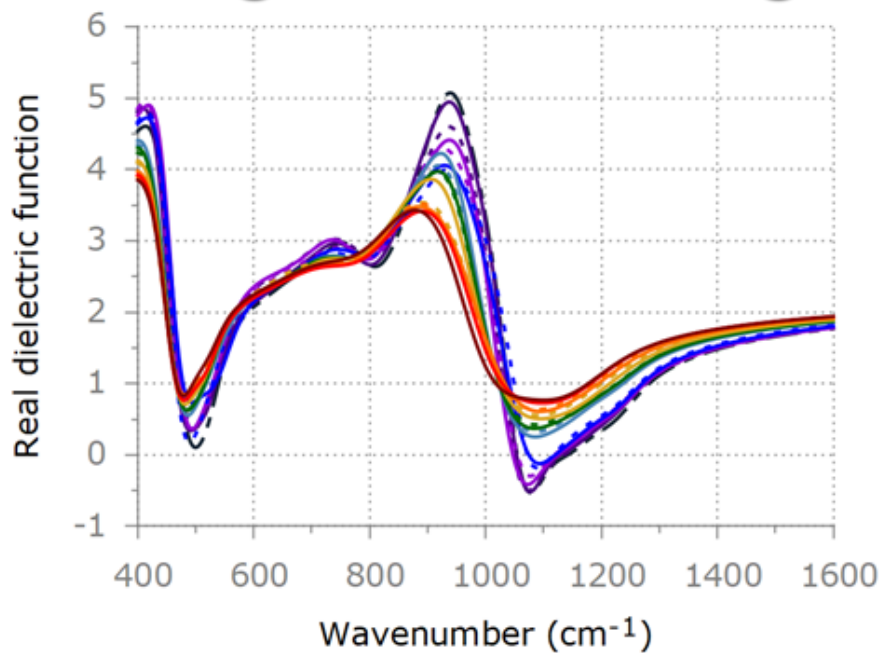
Silicate glass containing iron



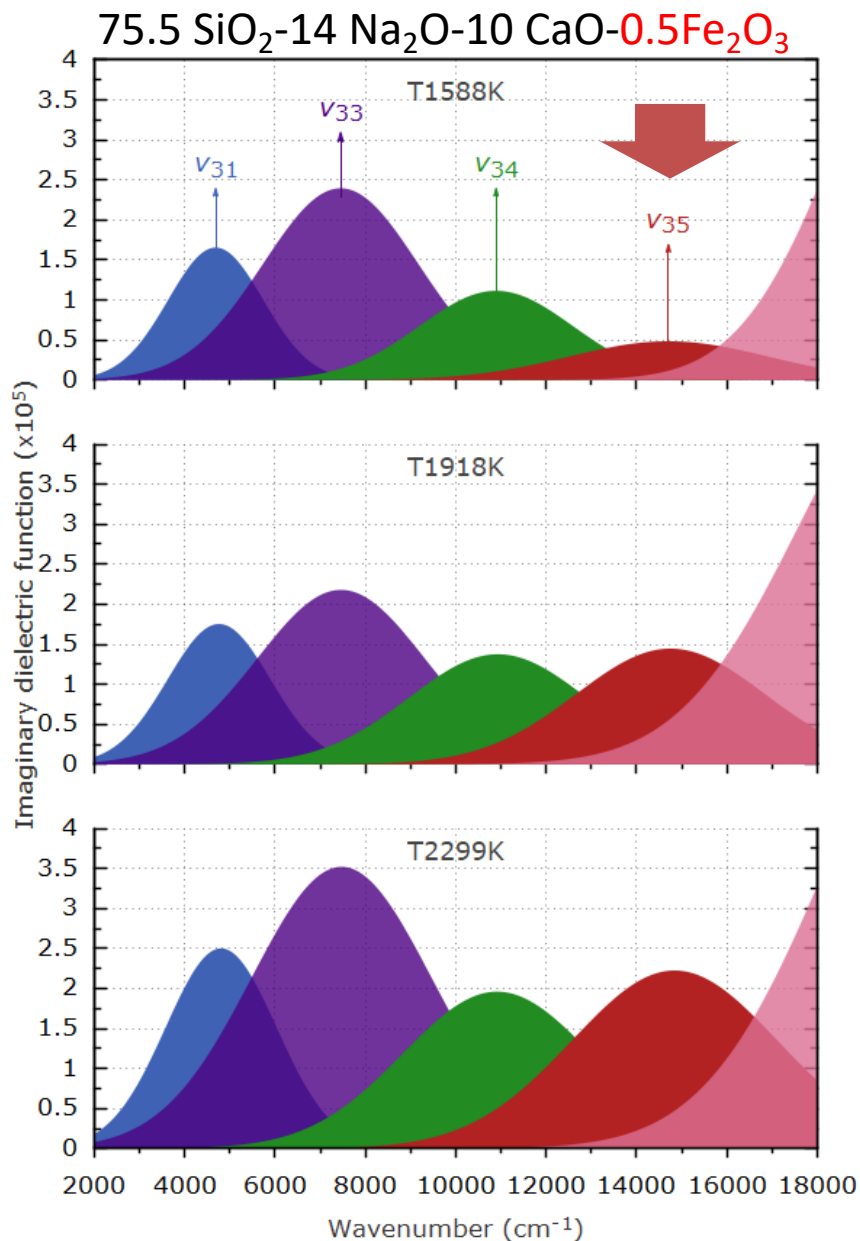
Vincent Vercamer. [REF-Vercamer]
Spectroscopic and Structural Properties of Iron in Silicate Glasses.
Material chemistry. Université Pierre et Marie Curie - Paris VI, 2016

Silicate glasses containing iron

75.5 SiO₂-14 Na₂O-10 CaO-0.5Fe₂O₃



Silicate glasses containing iron



Fit of Fe²⁺ bands with 3 Gaussian functions for NCS05Red [REF-Vercamer]

	Position (cm ⁻¹)	σ (cm ⁻¹)	FWHM (cm ⁻¹)	Intensity (cm ⁻¹)	$\epsilon_{\text{Fe}^{2+}}$ (L/mol/cm)	Area (cm ⁻²)
NCS05Red fit3						
#1	4848	492	1159	0.75	4.8	651.6
#2	7812	1277	3007	0.96	6.2	2181.4
#3	9775	3177	7482	3.65	23.7	20557.5

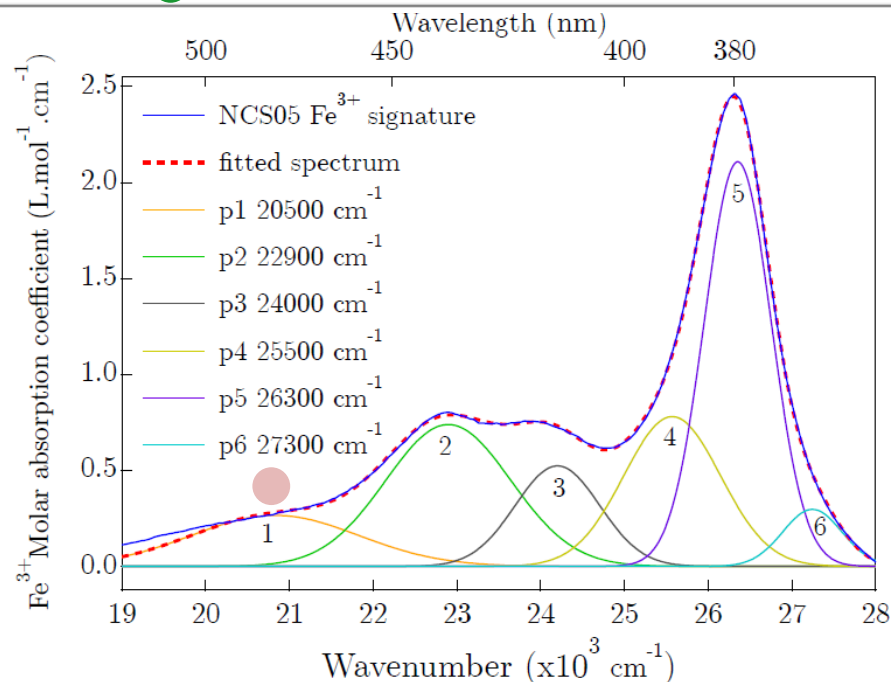


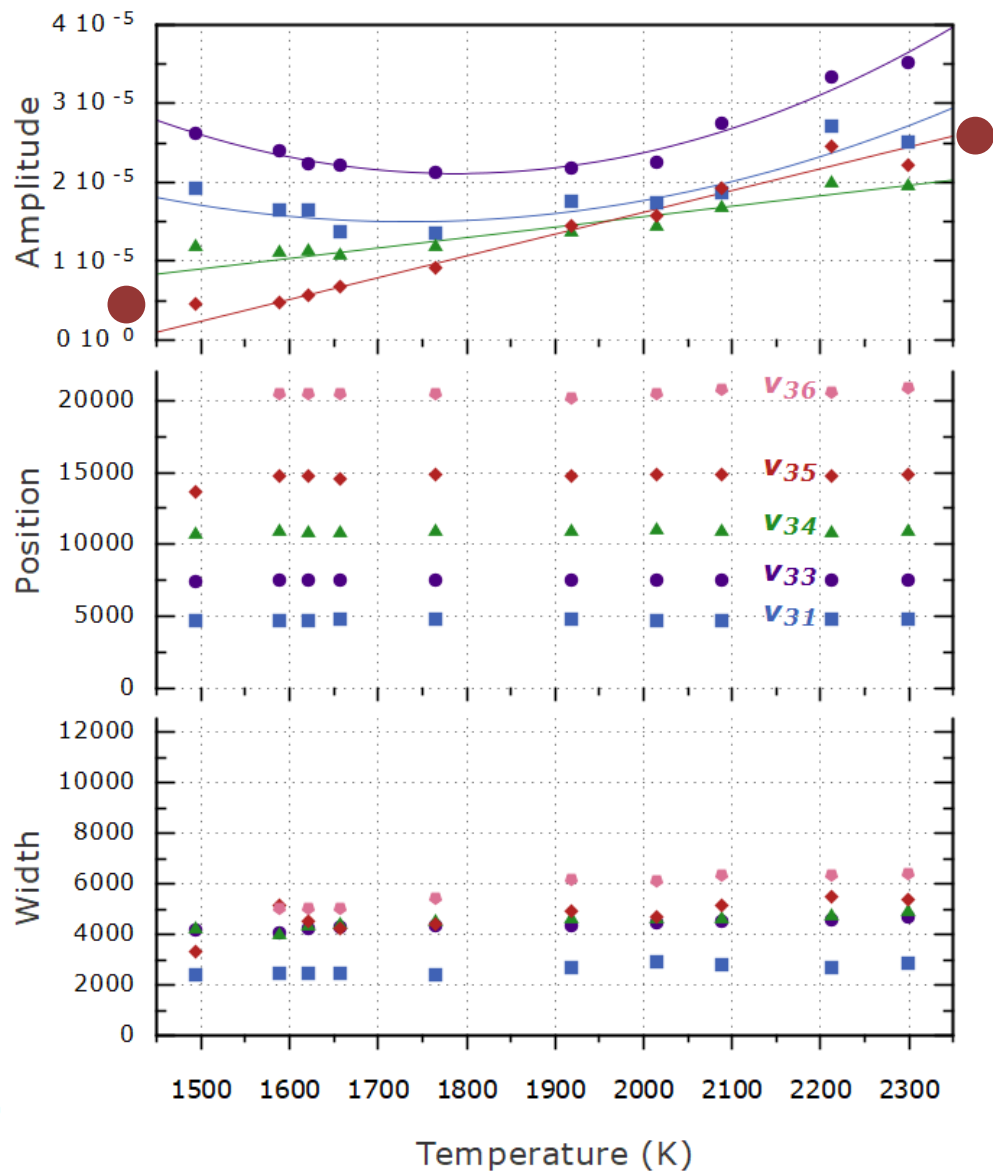
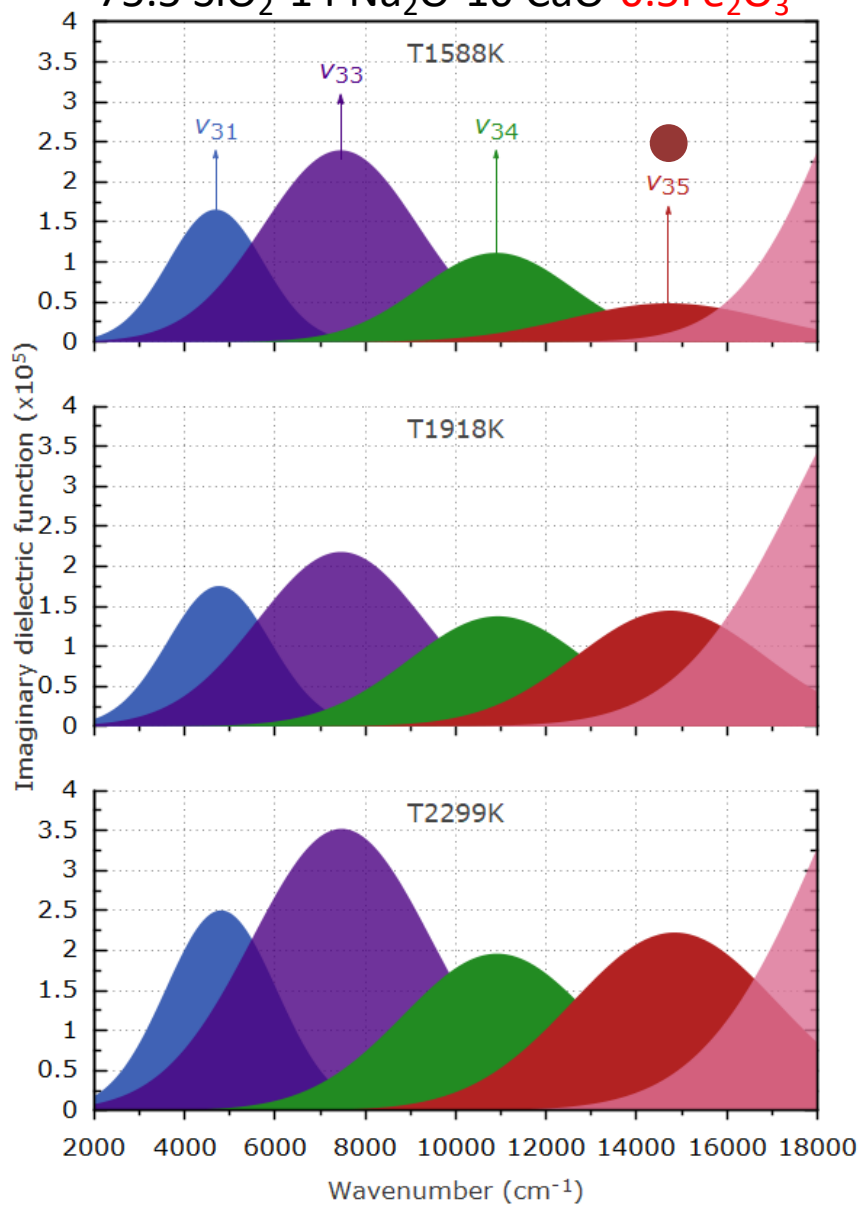
Figure 5.15 – Molar absorption coefficient of Fe³⁺ in the soda-lime oxidized glass (NCS05Ox) after UV-edge removal. Example of Fe³⁺ bands fitted with 6 Gaussians.

Intervalence Charge Transfer (IVCT) ●

Transfer of an electron between two adjacent Fe²⁺-Fe³⁺ ions.
Strong increase at high temperature in the melt

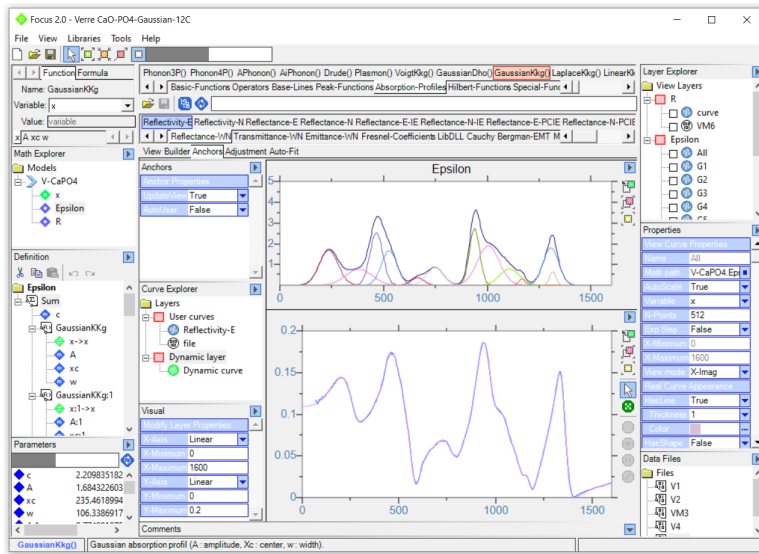
Silicate glasses containing iron

75.5 SiO₂-14 Na₂O-10 CaO-0.5Fe₂O₃

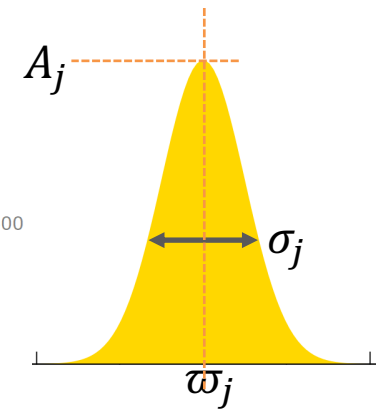
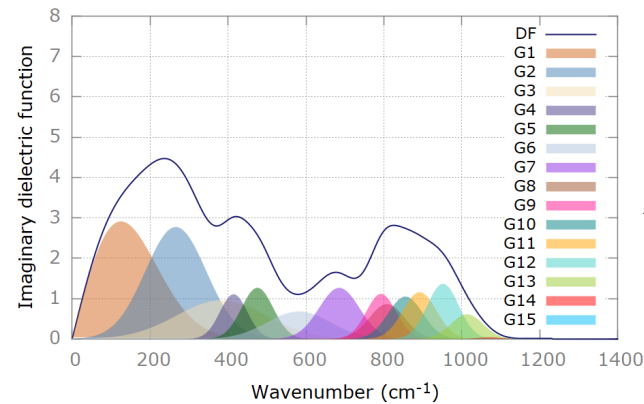


Conclusion

Infrared spectroscopy is a powerful tool to investigate the structural and optical properties of glasses and melts at high temperature.



Infrared spectroscopy practical



Thank you for your attention

