Combining neutron scattering with Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy

How multiple techniques can enhance our structural understanding

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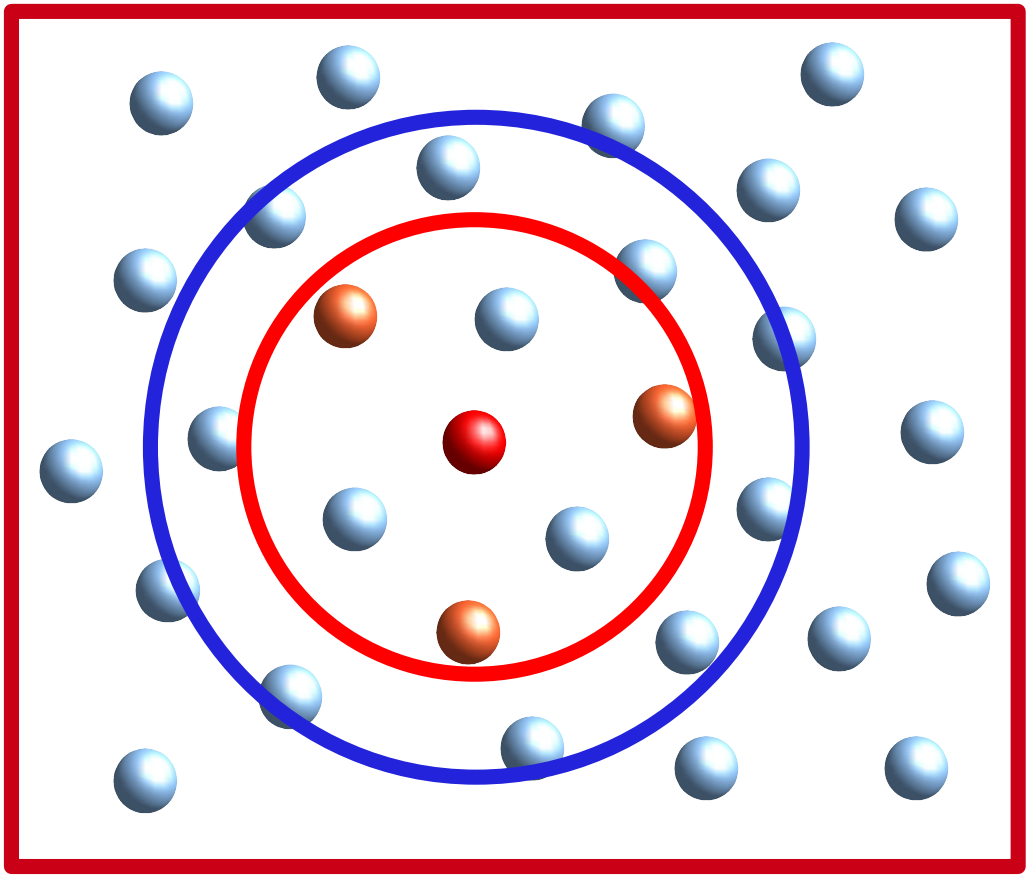
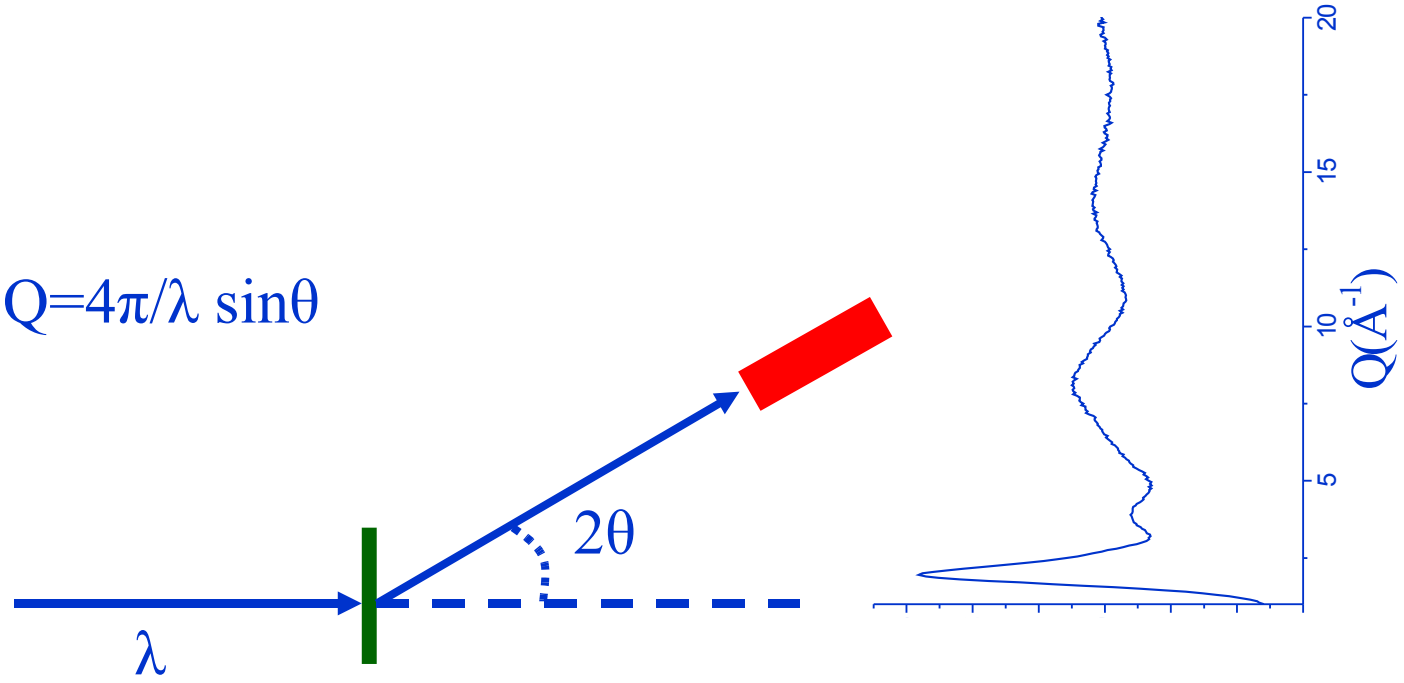
Structural probes of varying sensitivity

Bulk probes: X-ray and neutron scattering



Chemically specific local probes: EXAFS, Neutron scattering with isotopic substitution, Anomalous X-ray scattering

Schematic of a diffraction experiment



The neutron diffraction experiment

Total Structure Factor

Atomic concentrations and scattering lengths

$$F(Q) = \sum_{\alpha,\beta} c_\alpha c_\beta b_\alpha b_\beta (S_{\alpha\beta}(Q) - 1)$$

Partial Structure Factors

$$S_{\alpha\beta}(Q) - 1 = 4\pi\rho \int_0^\infty r^2 (g_{\alpha\beta}(r) - 1) \frac{\sin(Qr)}{Qr} dr$$

Atomic density

Partial Pair Distribution Functions

Structure and pairwise atomic correlations

$$\frac{n(n+1)}{2}$$

Number of distinct atom types	Number of pair terms
1	1
2	3
3	6
4	10
....	....
9	45
10	55

SiO_2

Si – Si
Si – O
O - O

Ag_3PO_4

Ag – Ag
Ag – P
Ag – O
P – P
P – O
O – O

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The structure of silica glass: an under-determined problem

$$F_{SiO_2}(Q) = c_{Si}^2 b_{Si}^2 [S_{SiSi}(Q) - 1] + 2c_{Si}c_O b_{Si} b_O [S_{SiO}(Q) - 1] + c_O^2 b_O^2 [S_{OO}(Q) - 1]$$

By neutrons: No isotopic variation in scattering length of silicon or oxygen

By X-rays: Silicon and oxygen absorption edges at too low an energy to make feasible anomalous X-ray scattering techniques

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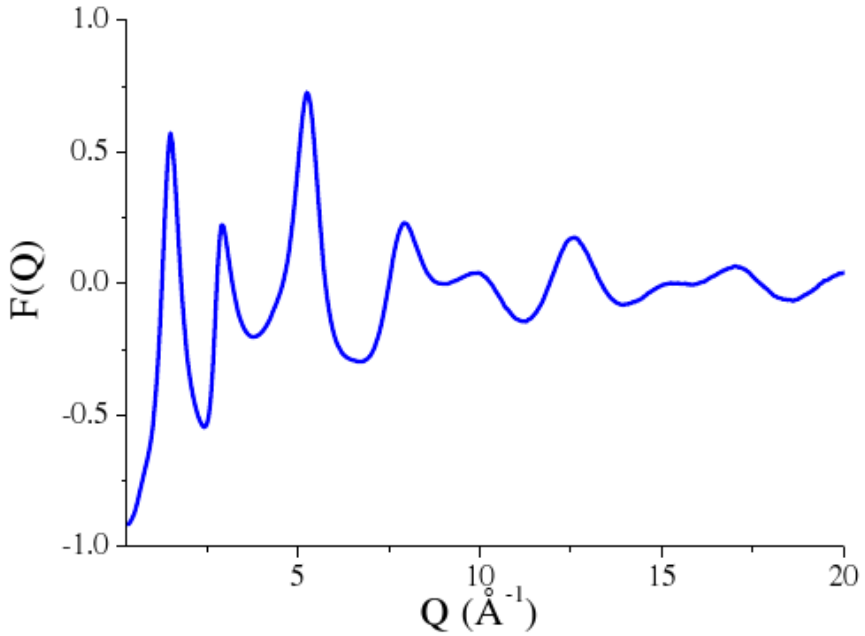
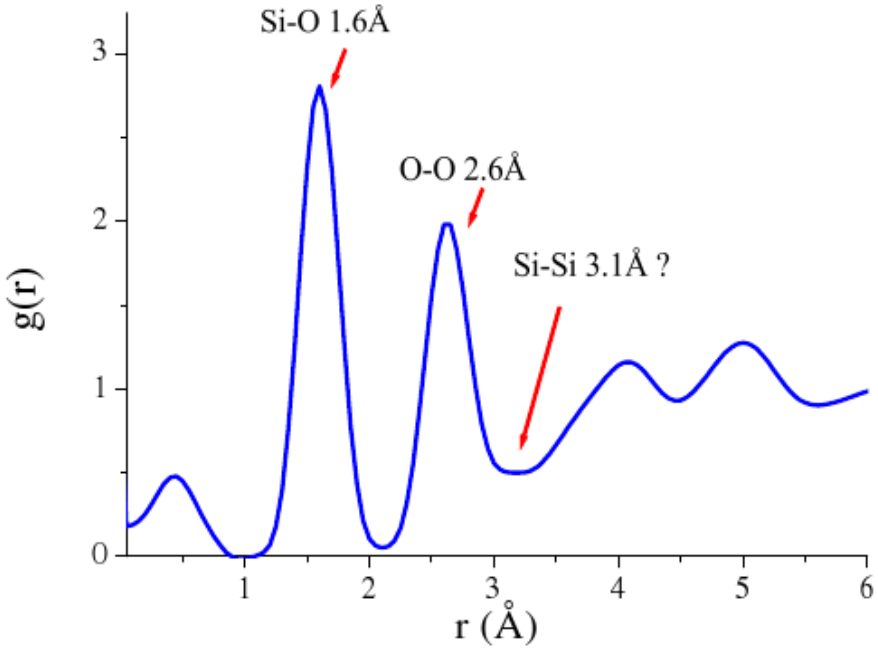
The neutron total structure factor and radial distribution function for silica





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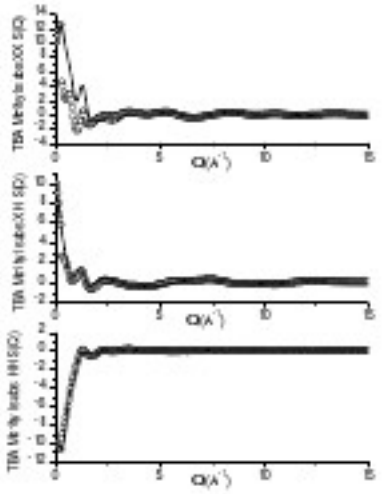
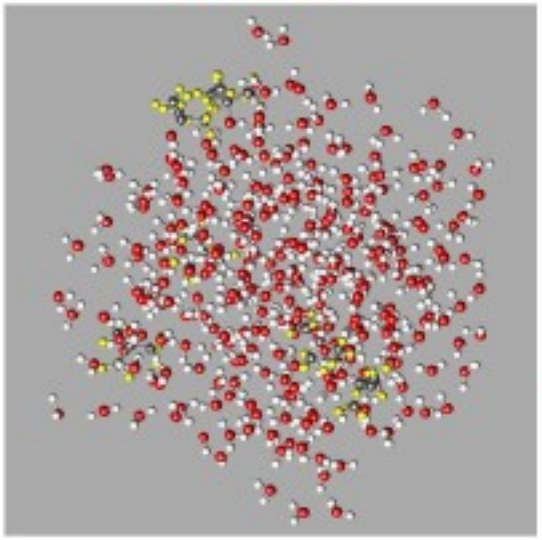
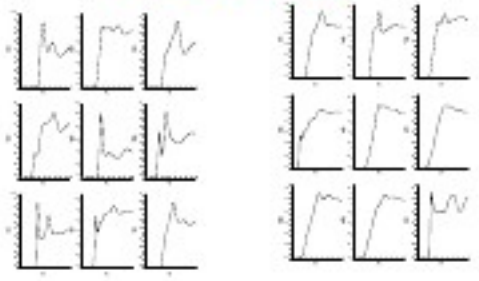
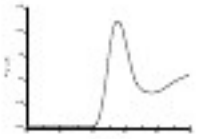
Empirical Potential Structure Refinement

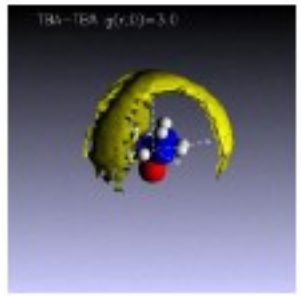
INPUT ***EPSR*** ***OUTPUT***











Constraints such as:
Density
Molecular geometry

$$U_{Total} = U_{reference} + U_{empirical\_potential}$$

$$\Delta S_{\alpha\beta}(Q) = S^{exp}_{\alpha\beta}(Q) - S^{sim}_{\alpha\beta}(Q)$$

$$U^{N+1}_{empirical} = U^{N}_{empirical} + \left(k_B T \times F.T.\left(\Delta S(Q)\right)\right)$$

A.K.Soper *Chem Phys* **202** p.295 (1996) & A.K.Soper *Phys Rev B* **72** 104204 (2005)

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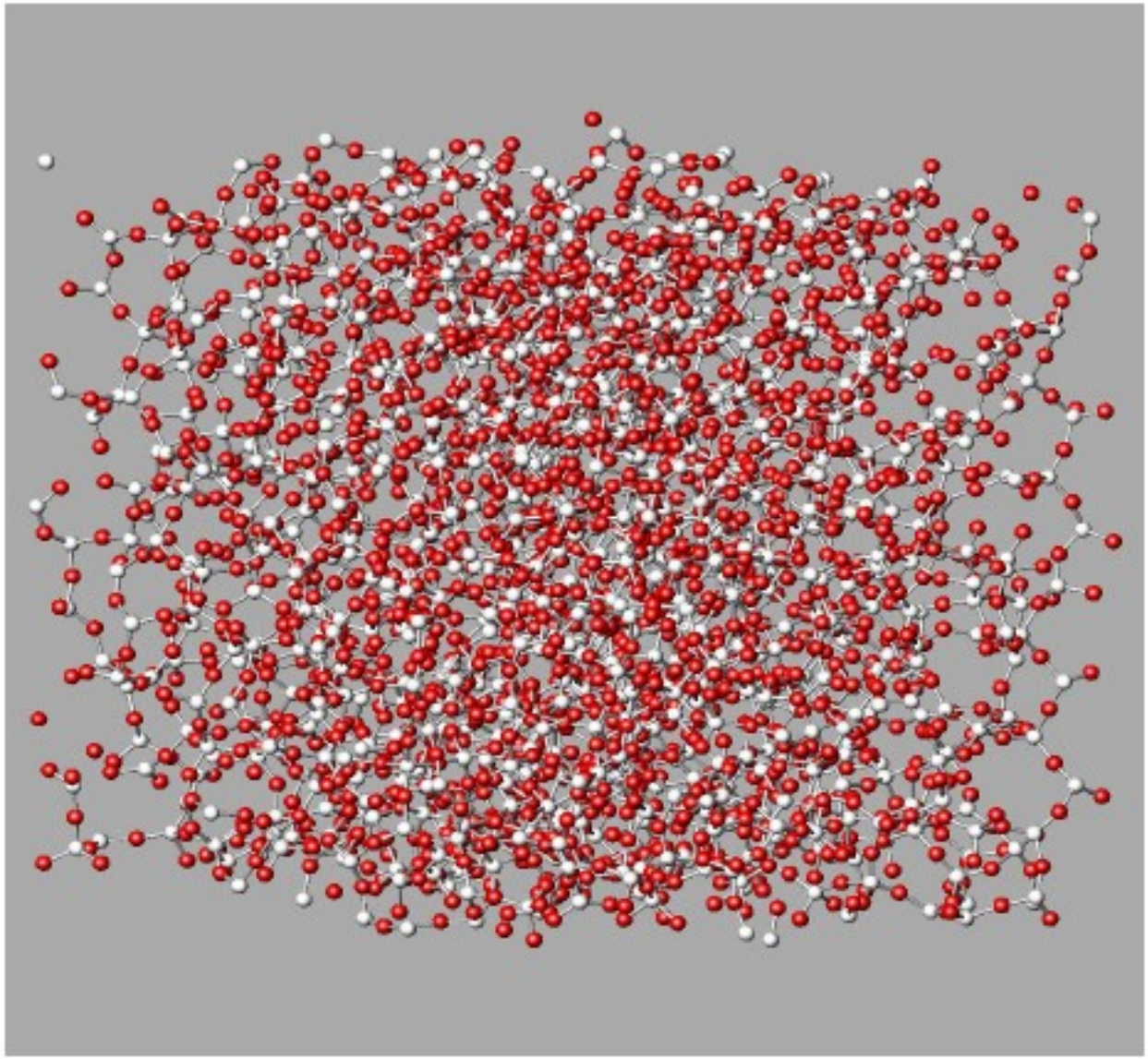
Silica simulation box

1000 Si atoms
2000 O atoms

Box side: 35.62Å

Density: 0.0664 ats/Å^3



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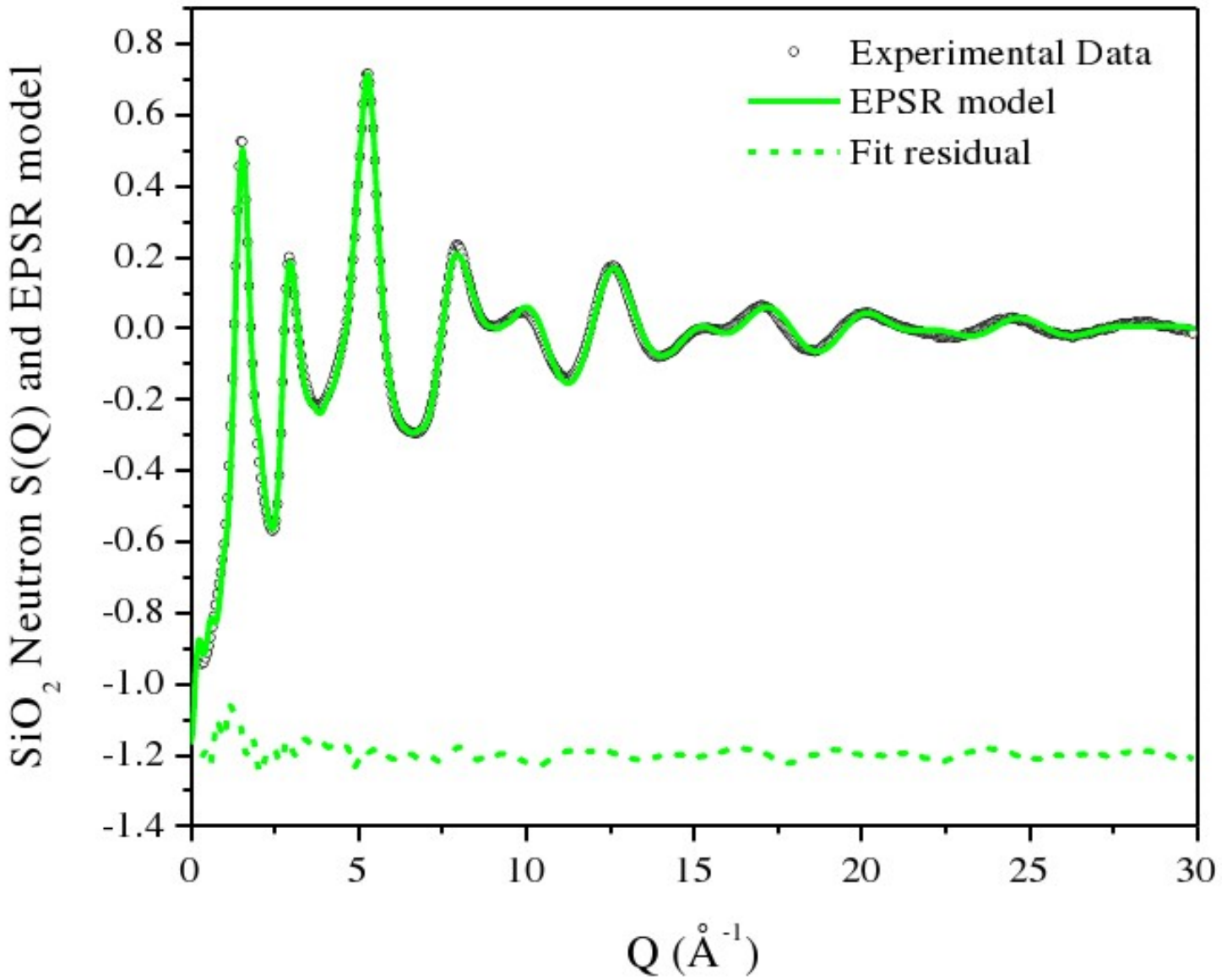
EPSR model fits to the neutron total structure factor for silica



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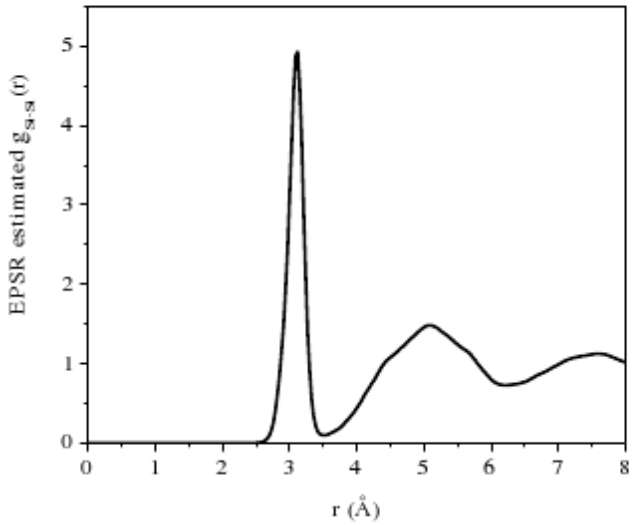
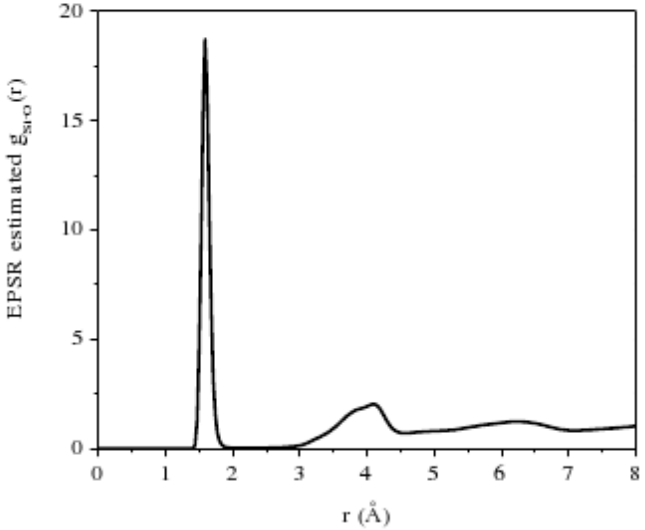
EPSR derived partial pair distribution functions

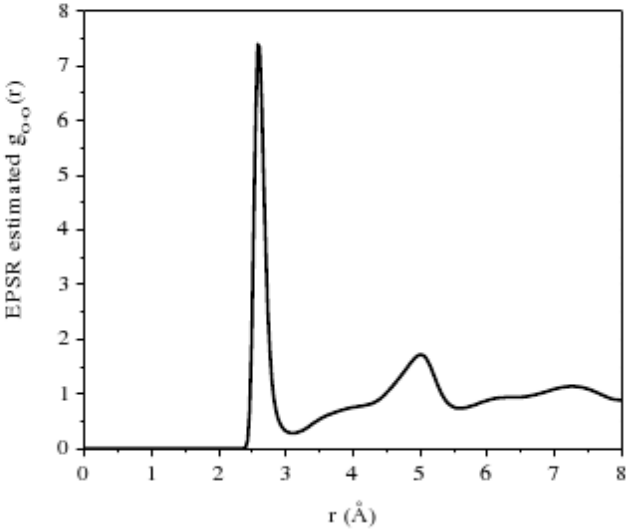
Si-Si



Si-O



O-O



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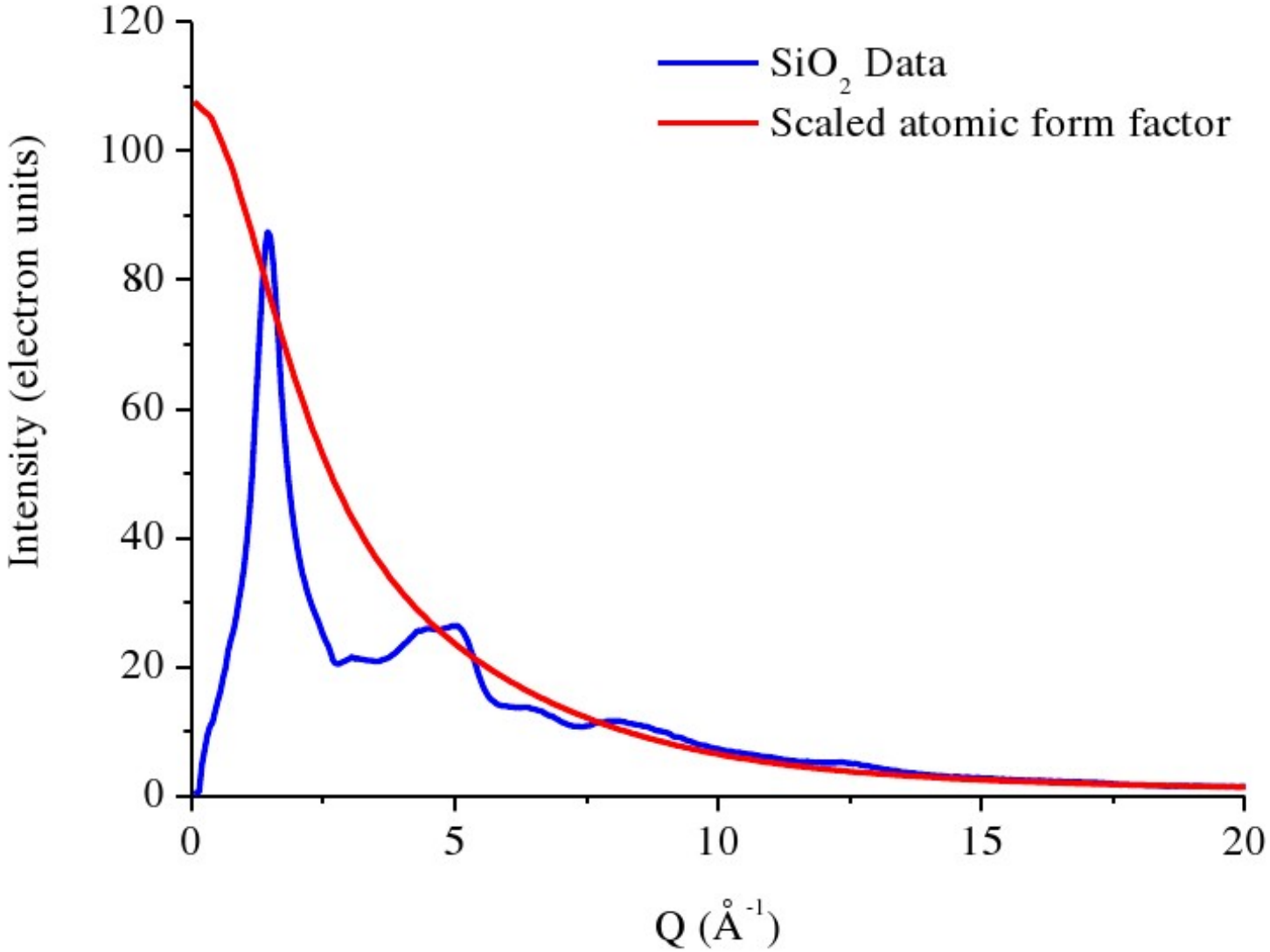
Testing the model – the X-ray total structure factor of silica



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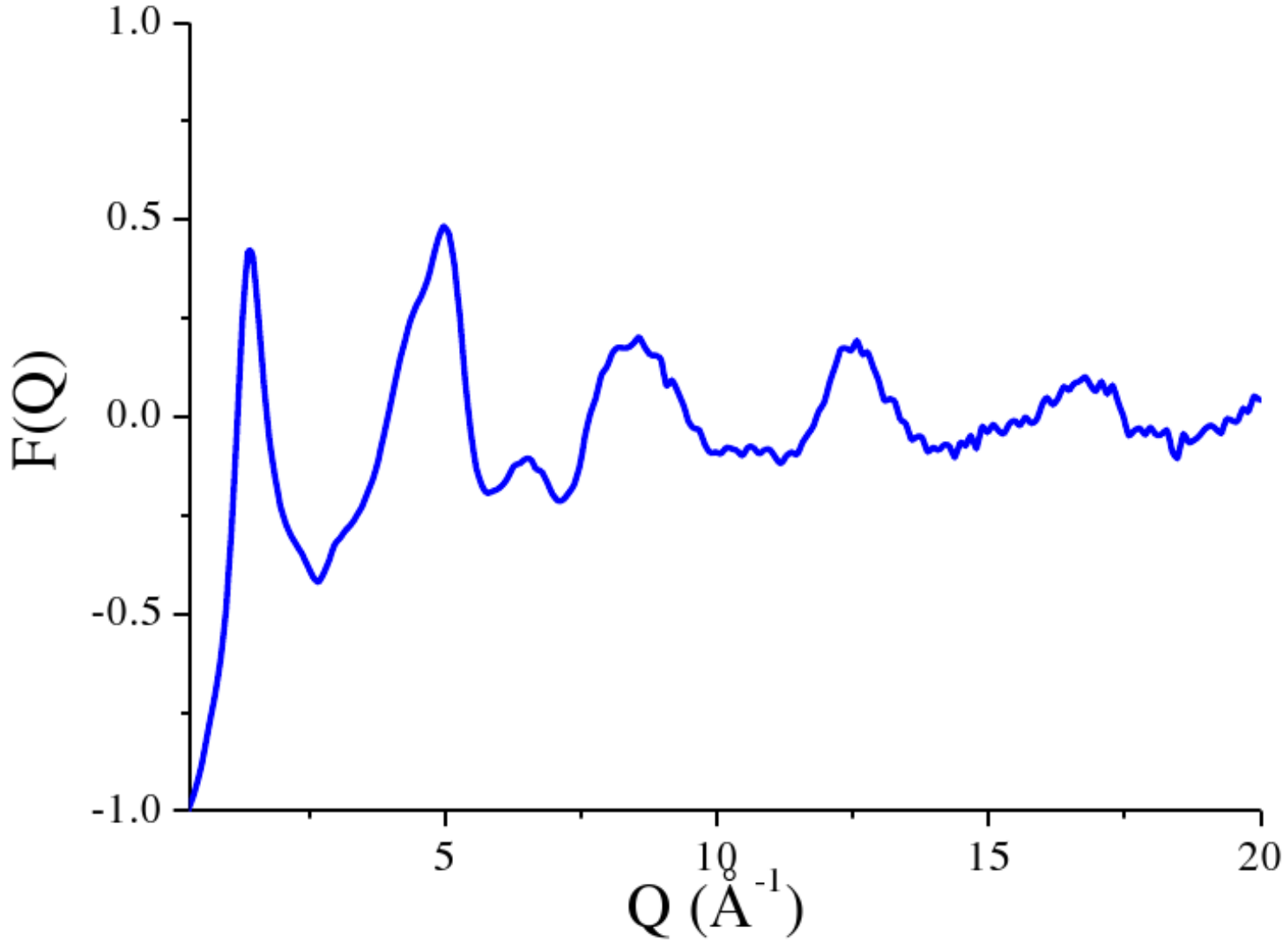

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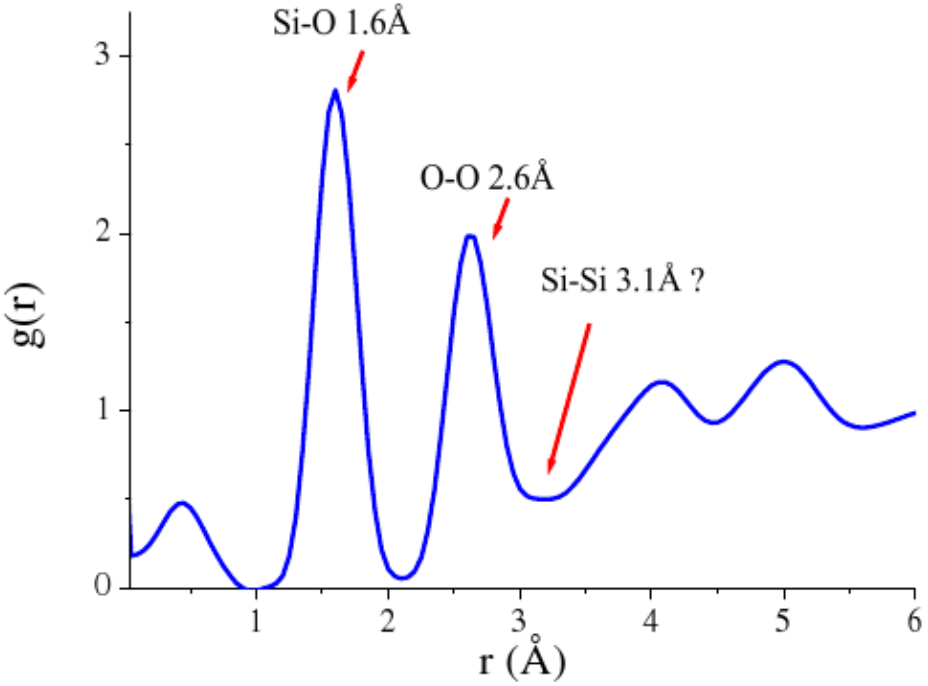
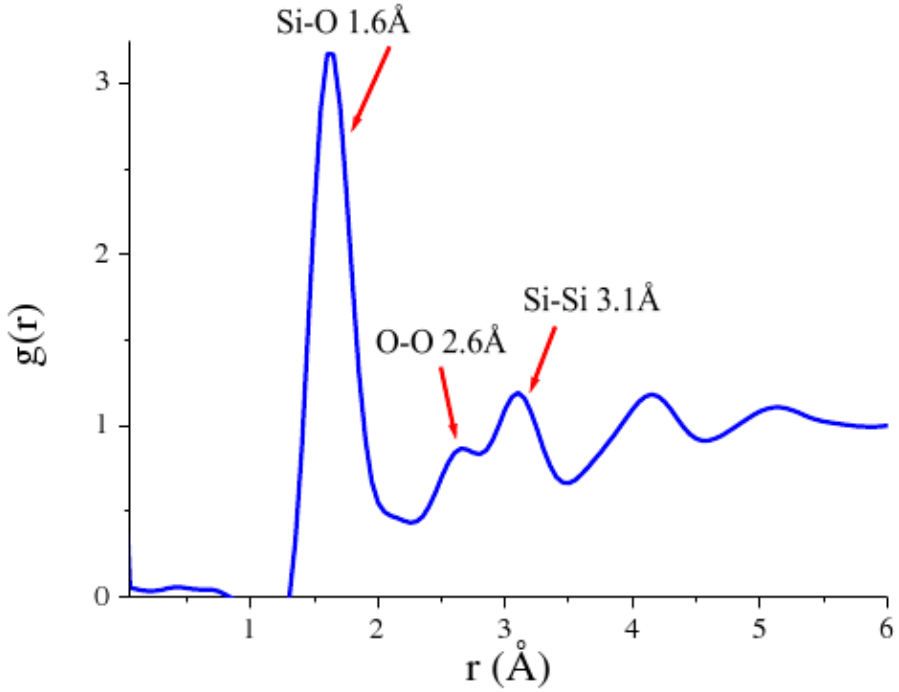
The neutron and X-ray total radial distribution functions for silica

Neutron



X-ray



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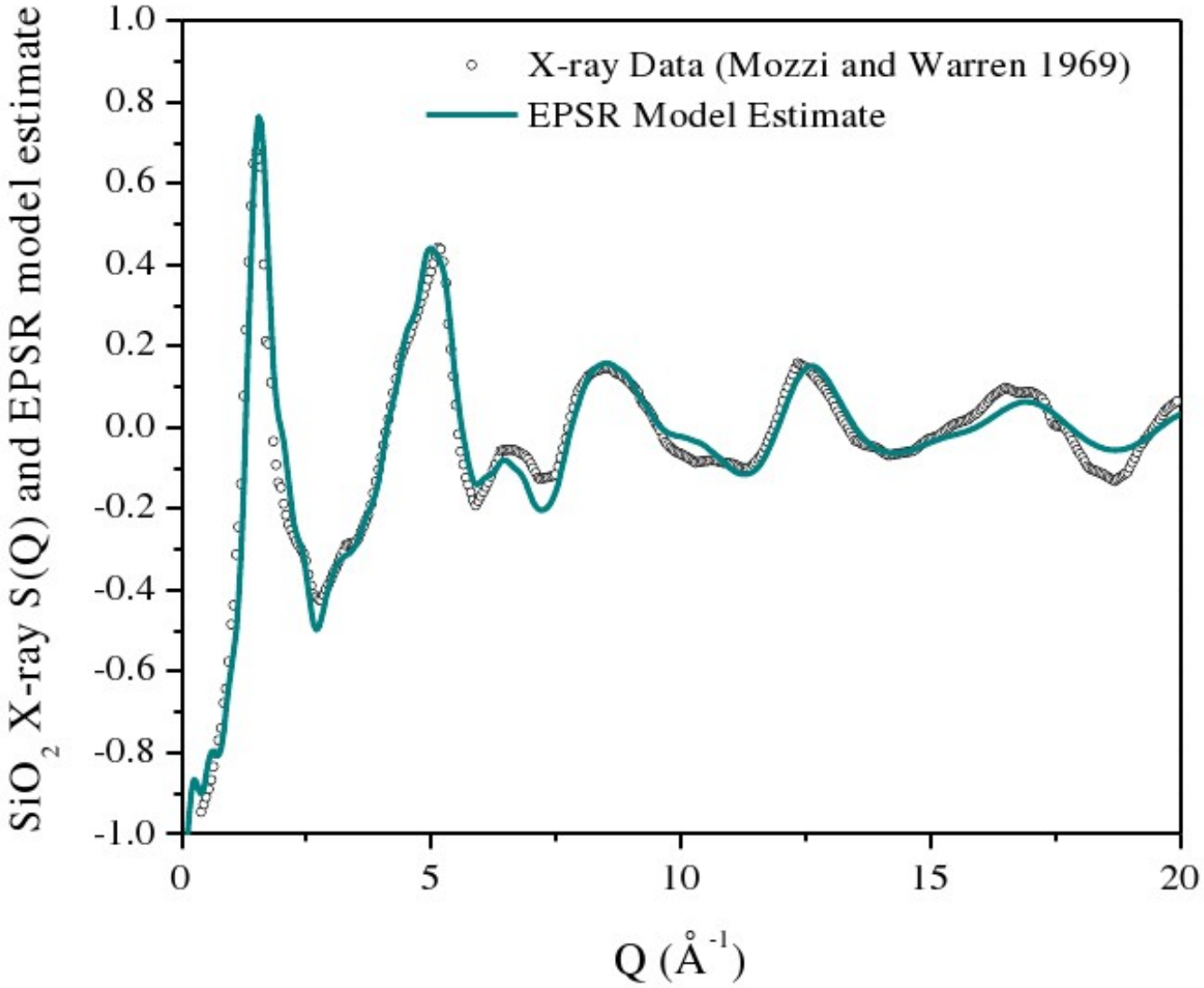
EPSR prediction for the X-ray total structure factor for silica



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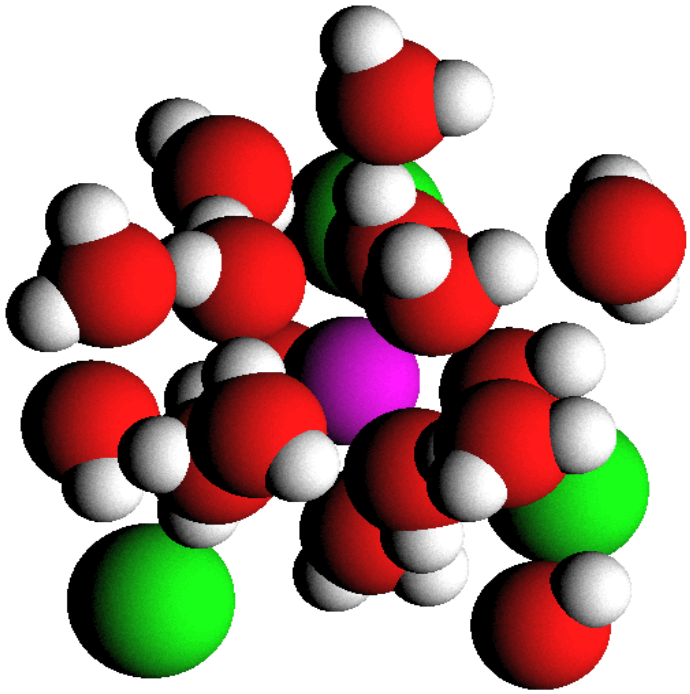
Structure of aqueous electrolyte solutions



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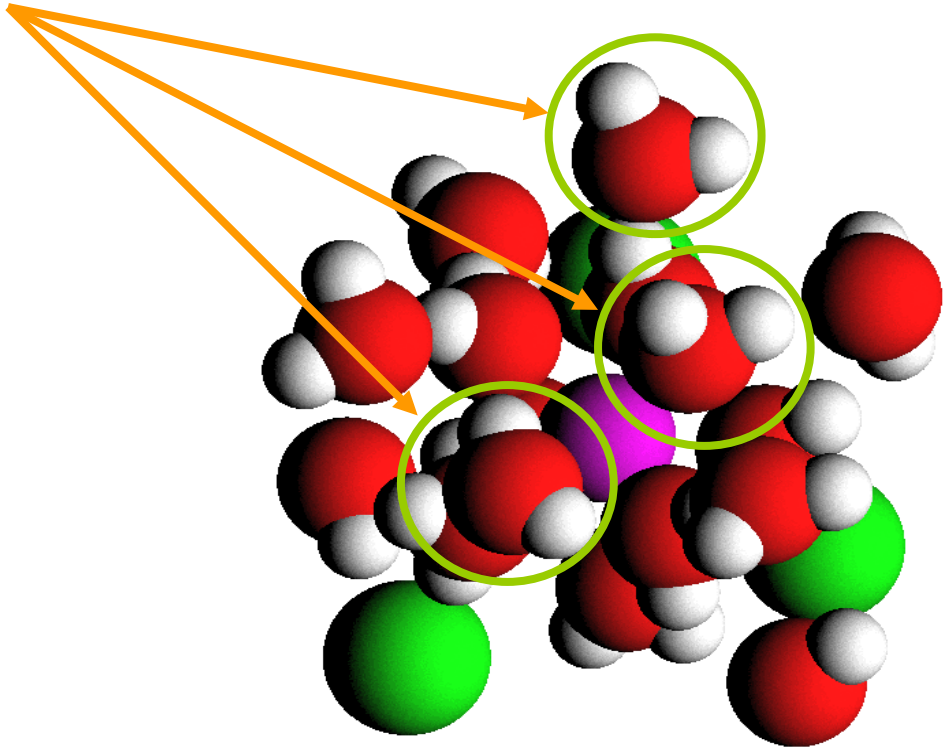
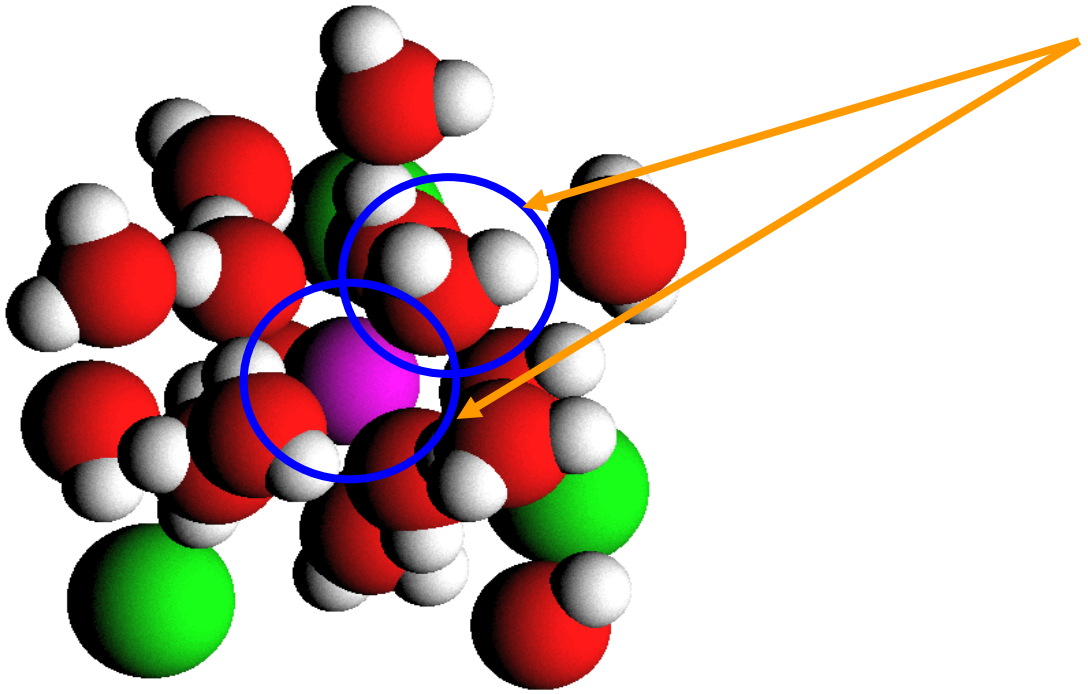
Structure of aqueous electrolyte solutions

Solvent-solvent interactions



Structure of aqueous electrolyte solutions

Cation-solvent interactions



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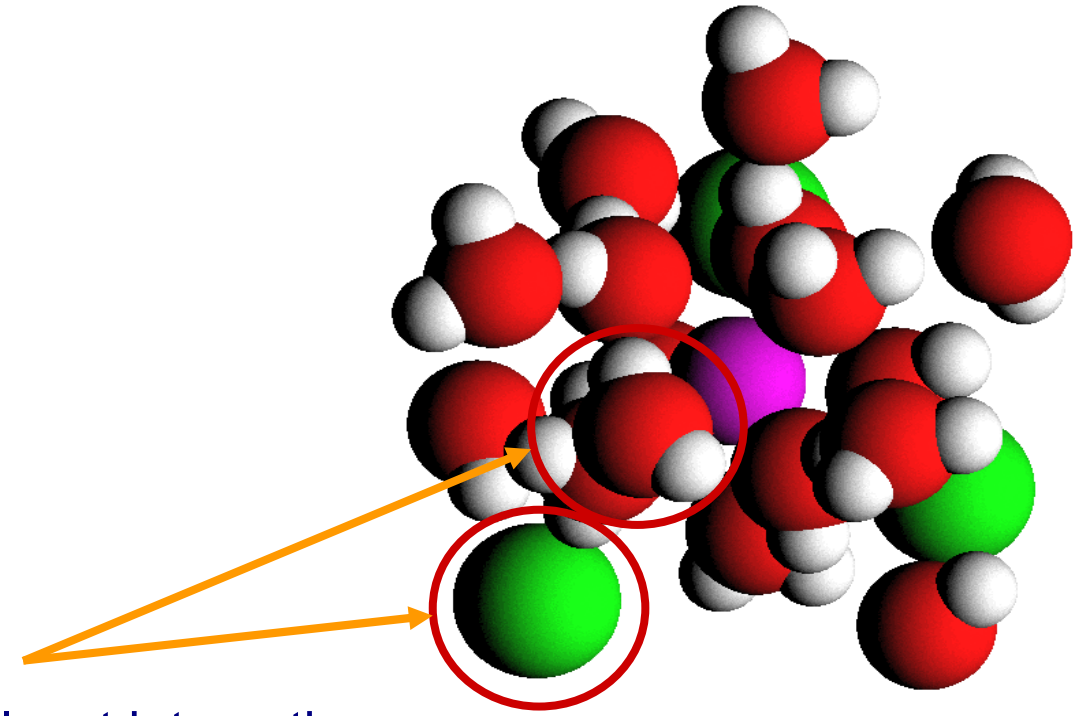
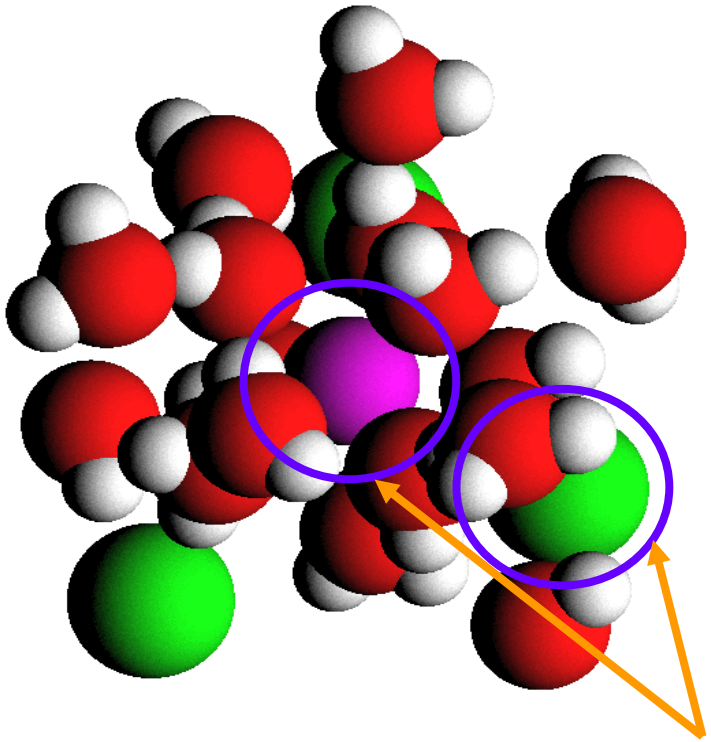
Structure of aqueous electrolyte solutions



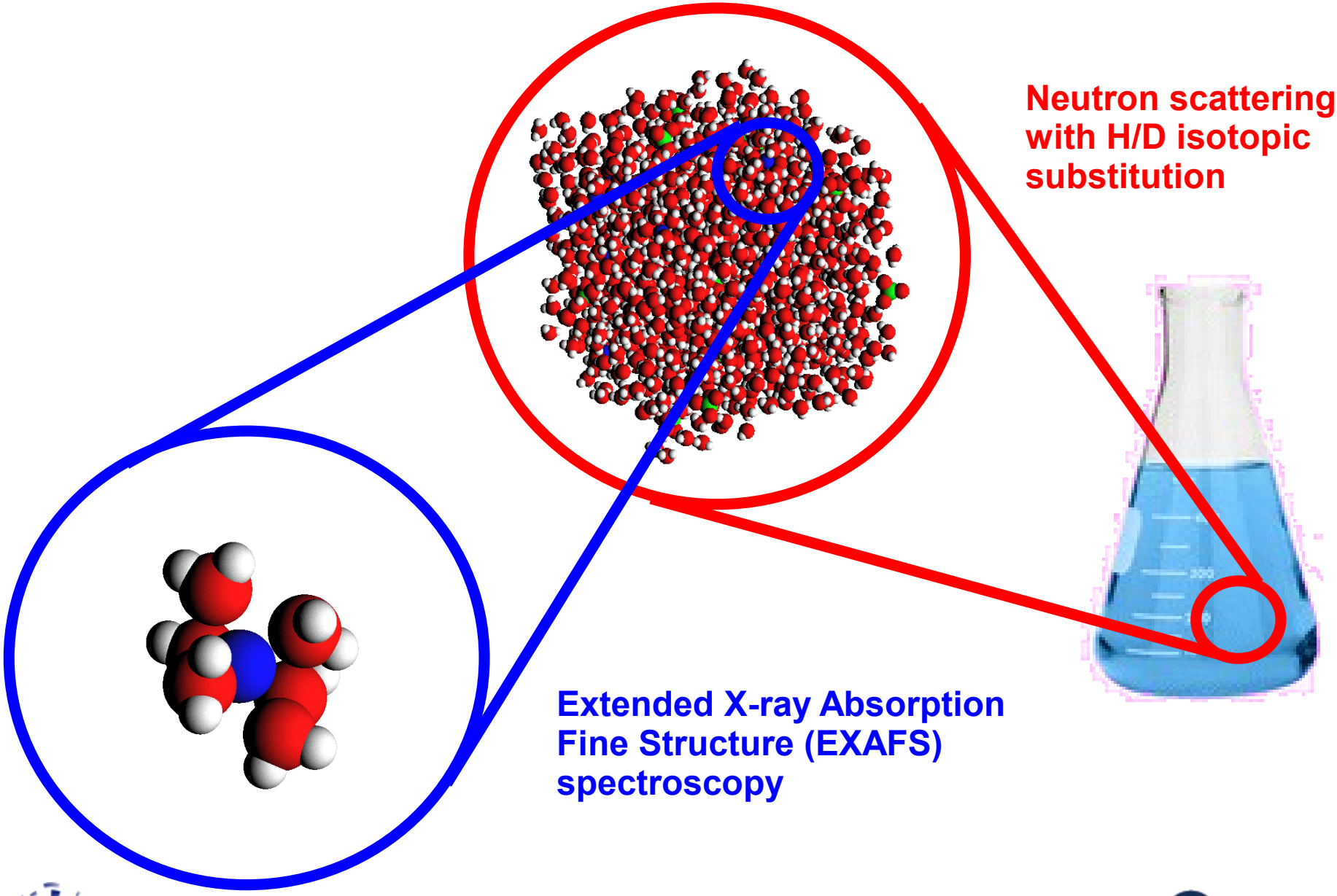
Anion-solvent interactions

Structure of aqueous electrolyte solutions



Cation-anion interactions

Aim to build 3D structural model consistent with experimental data



Neutron scattering with H/D isotopic substitution

Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy

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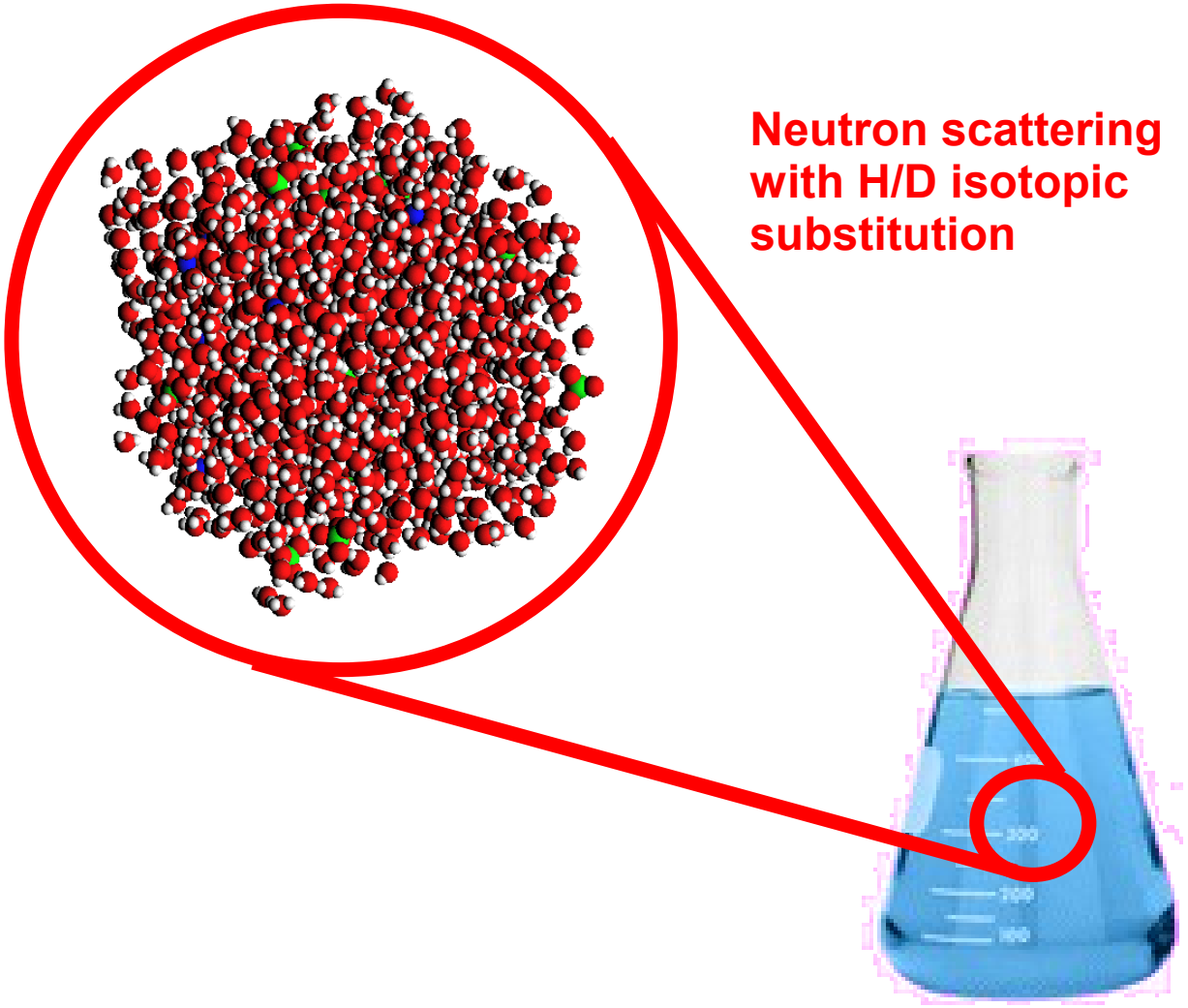
Step 1: structure of the bulk solution by neutron scattering methods



Neutron scattering with H/D isotopic substitution

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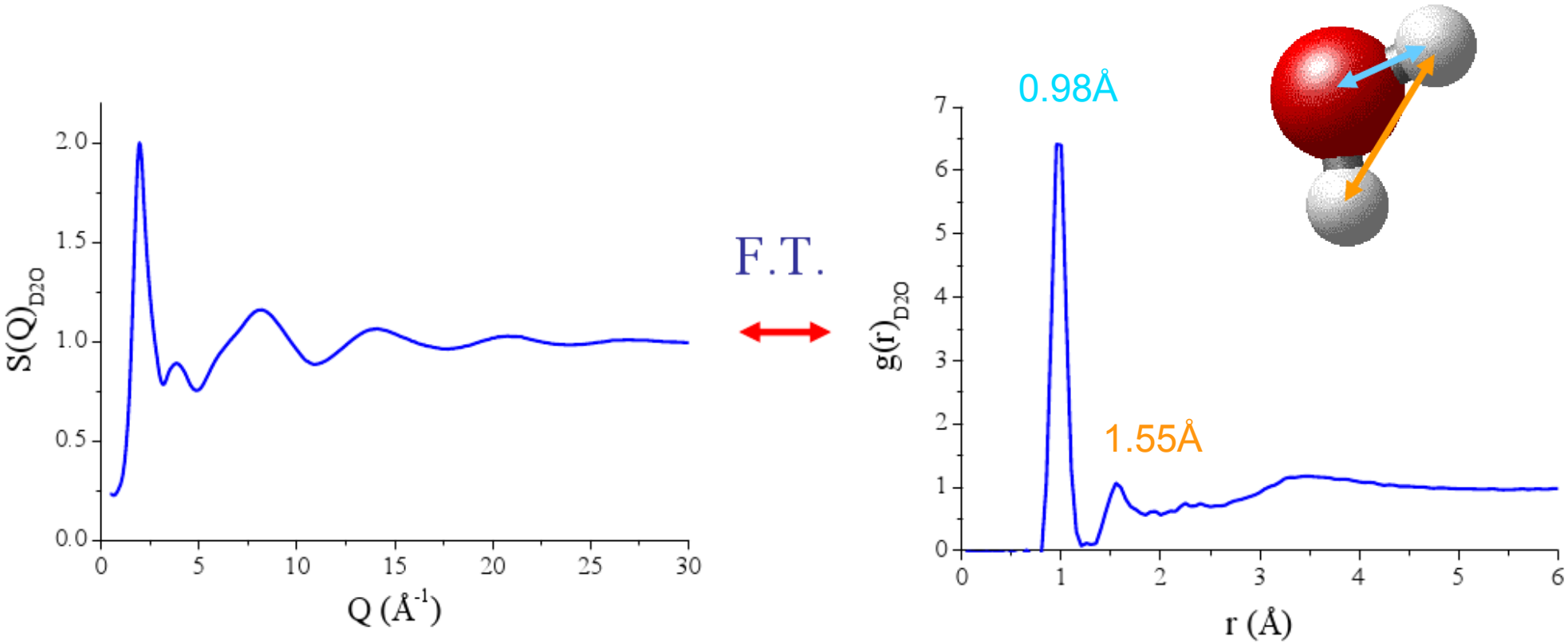
The neutron diffraction experiment without isotopic substitution



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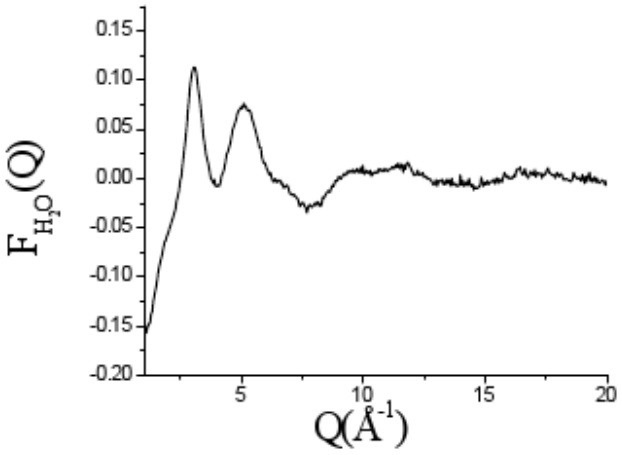
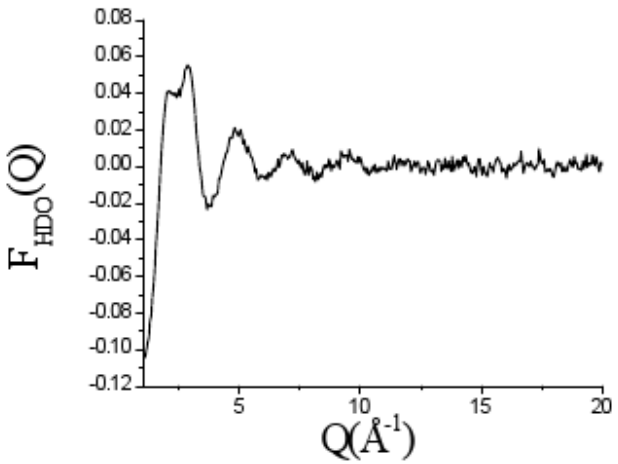
H/D isotopic substitution – the case of water

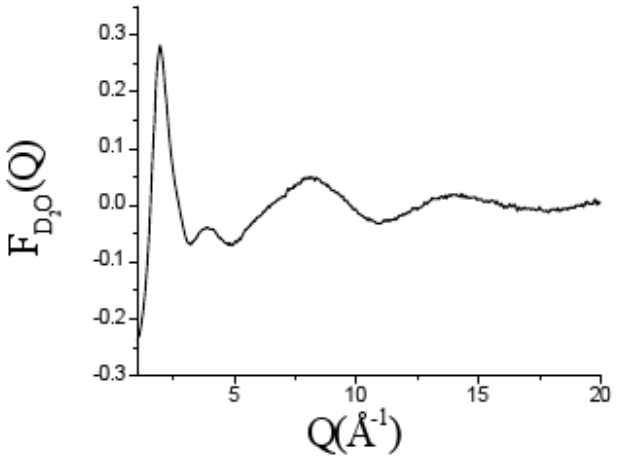
$$F_{H_2O}(Q)=c_X^2 b_X^2[S_{XX}(Q)-1]+2c_X b_X c_H b_H[S_{XH}(Q)-1]+c_H^2 b_H^2[S_{HH}(Q)-1]$$

$$F_{HDO}(Q)=c_X^2 b_X^2[S_{XX}(Q)-1]+2c_X b_X c_H b_{HD}[S_{XH}(Q)-1]+c_H^2 b_{HD}^2[S_{HH}(Q)-1]$$

$$F_{D_2O}(Q)=c_X^2 b_X^2[S_{XX}(Q)-1]+2c_X b_X c_H b_D[S_{XH}(Q)-1]+c_H^2 b_D^2[S_{HH}(Q)-1]$$







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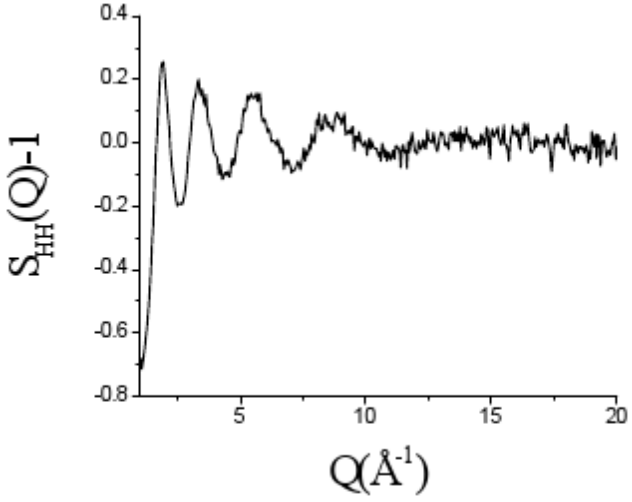
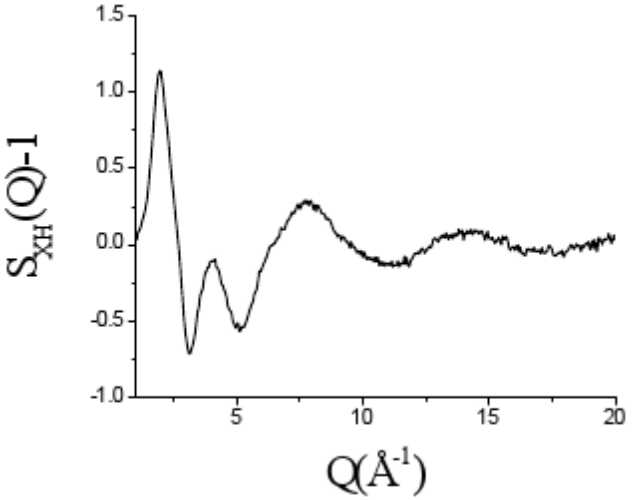
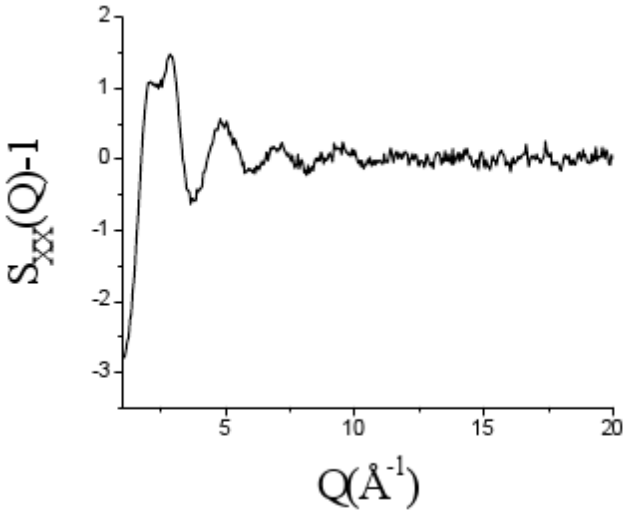
H/D isotopic substitution – the case of water

$$S_{HH}(Q)-1=\frac{(xF_H(Q)+(1-x)F_D(Q)-F_{HD}(Q))}{(c_H^2(xb_H^2+(1-x)b_D^2-b_{HD}^2))}$$

Etc.







$$S_{\alpha\beta}(Q)-1=4\pi\rho\int r^2[g_{\alpha\beta}(r)-1]\frac{\sin(Qr)}{Qr}dr$$

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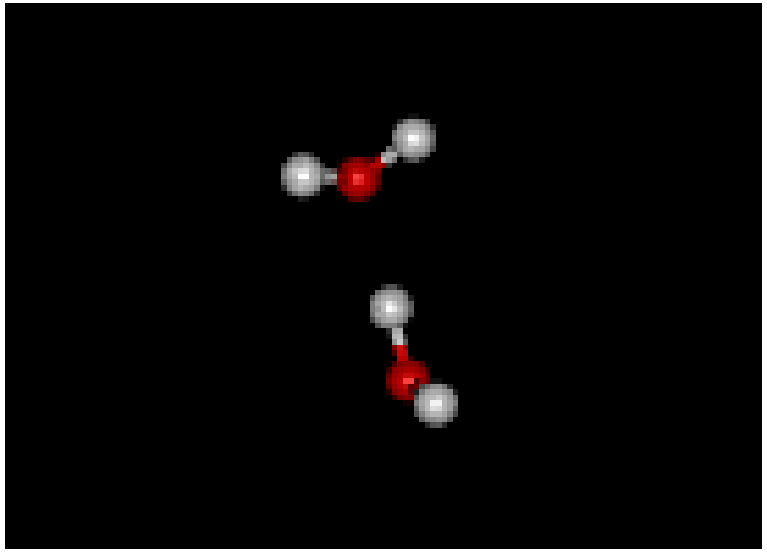
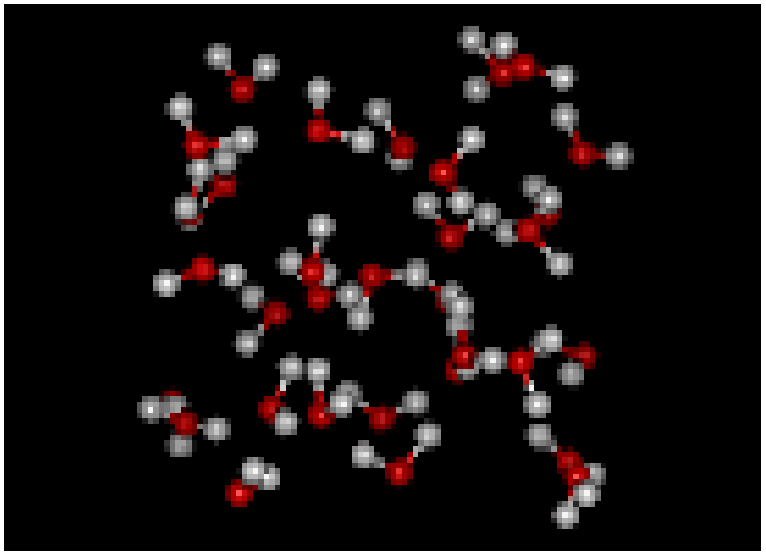
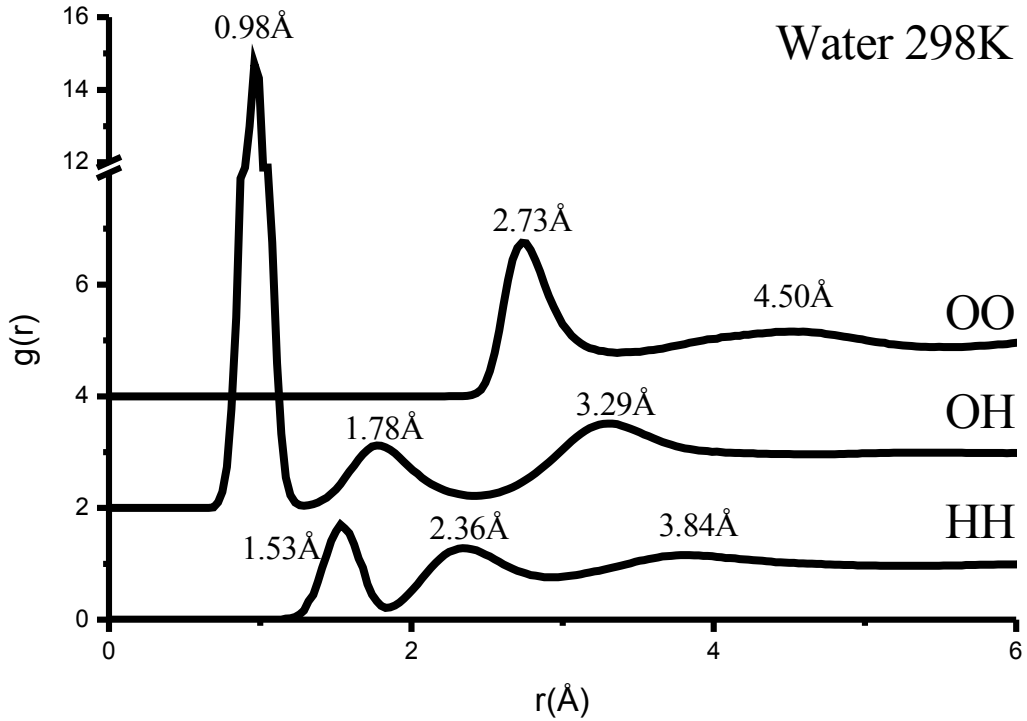
H/D isotopic substitution – the case of water







Access to distances and angles

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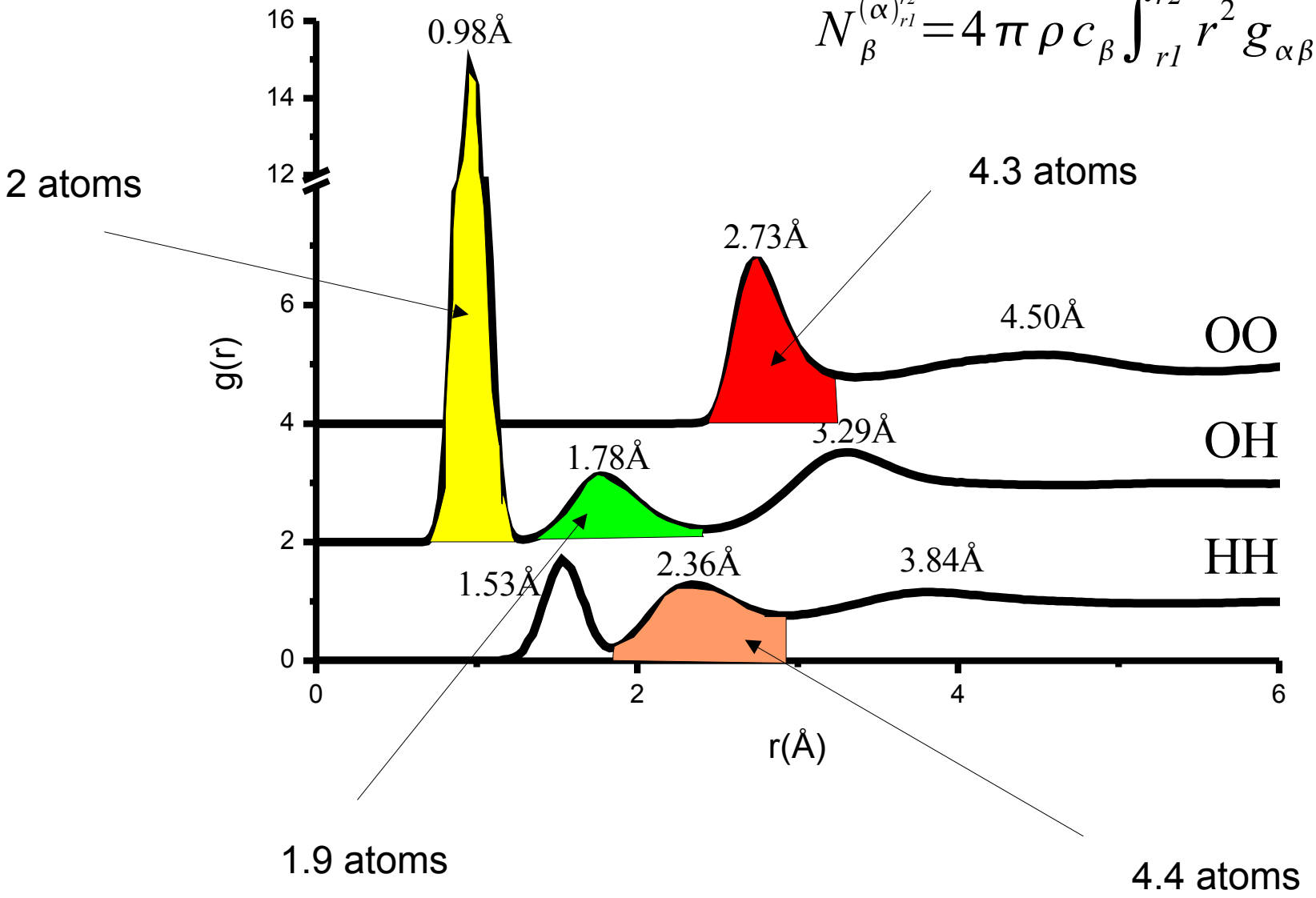
H/D isotopic substitution – the case of water

$$N_{\beta}^{(\alpha)_{r1}^{r2}} = 4\pi\rho c_{\beta}\int_{r1}^{r2} r^2 g_{\alpha\beta}(r)\,dr$$



Access to coordination numbers

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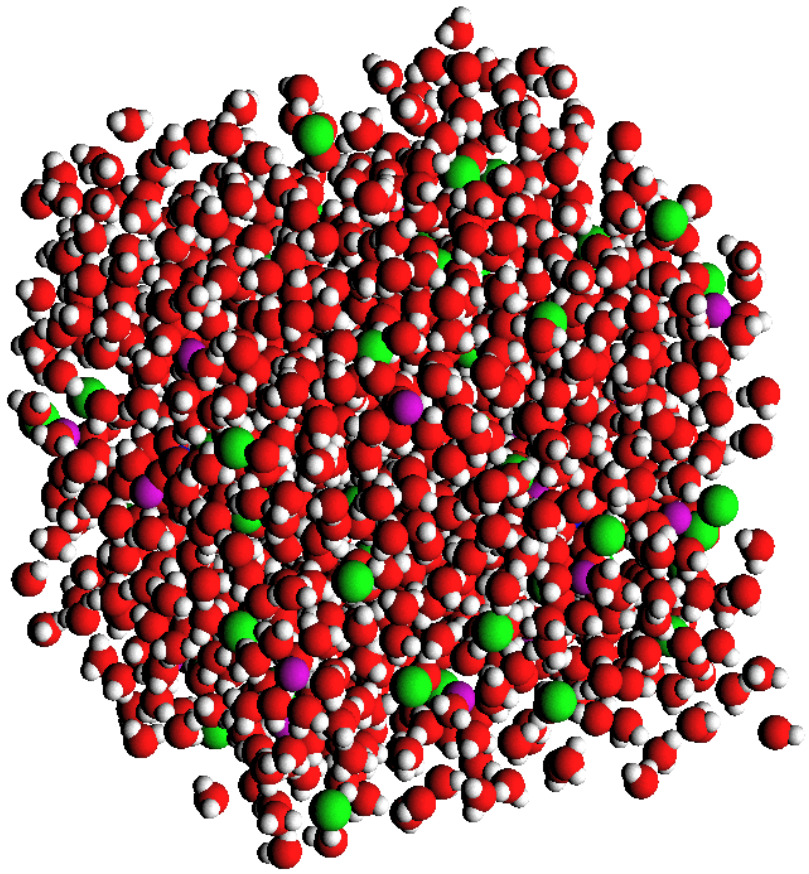
H/D isotopic substitution 1.0m YCl_3 in water



D2O solution weights	
Y - Y	0.004%
Y - Cl	0.036%
Y - OW	0.412%
Y - HW	0.951%
Cl - Cl	0.068%
Cl - OW	1.536%
Cl - HW	3.524%
OW - OW	8.603%
OW - HW	39.510%
HW - HW	45.355%

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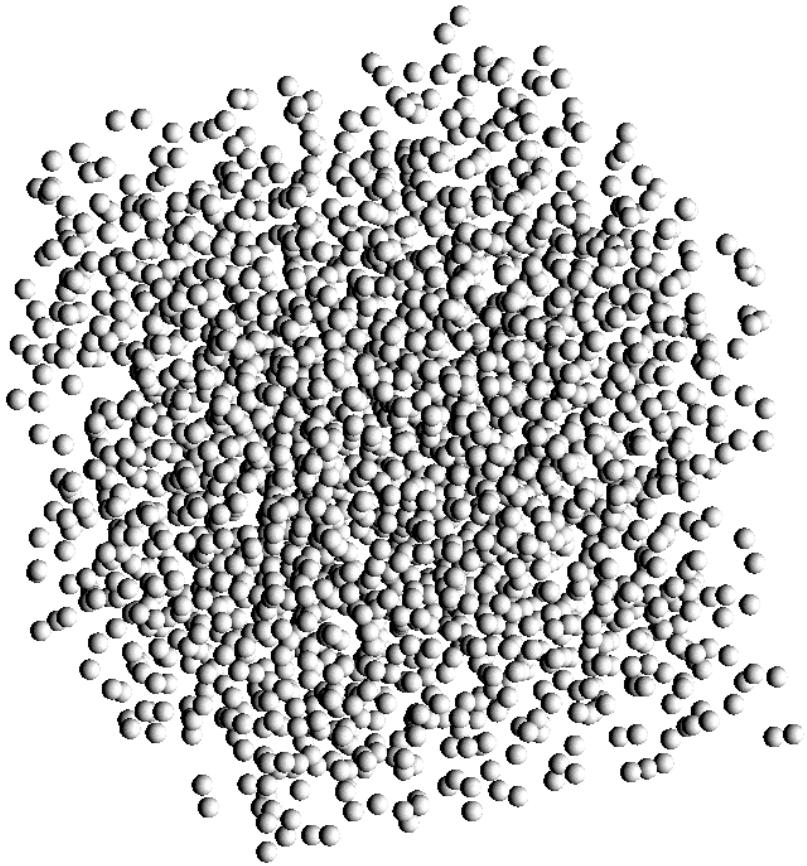
H/D isotopic substitution 1.0m YCl_3 in water



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Empirical Potential Structure Refinement

Monte Carlo simulation where the atomic interactions are governed by a reference potential plus a perturbation potential derived from experimental scattering data

$$U_{\alpha\beta}(r) = U_{\alpha\beta}^{(\mathrm{Ref})}(r) + U_{\alpha\beta}^{(\mathrm{EP})}(r)$$

Reference potential

$$U_{\alpha\beta}(r) = 4\varepsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r_{ij}}\right)^{6}\right] + \frac{q_\alpha q_\beta}{4\pi\varepsilon_0 r_{ij}} + U_{\alpha\beta}^{(\mathrm{EP})}(r)$$

Lennard-Jones + Coulomb + Empirical Potential

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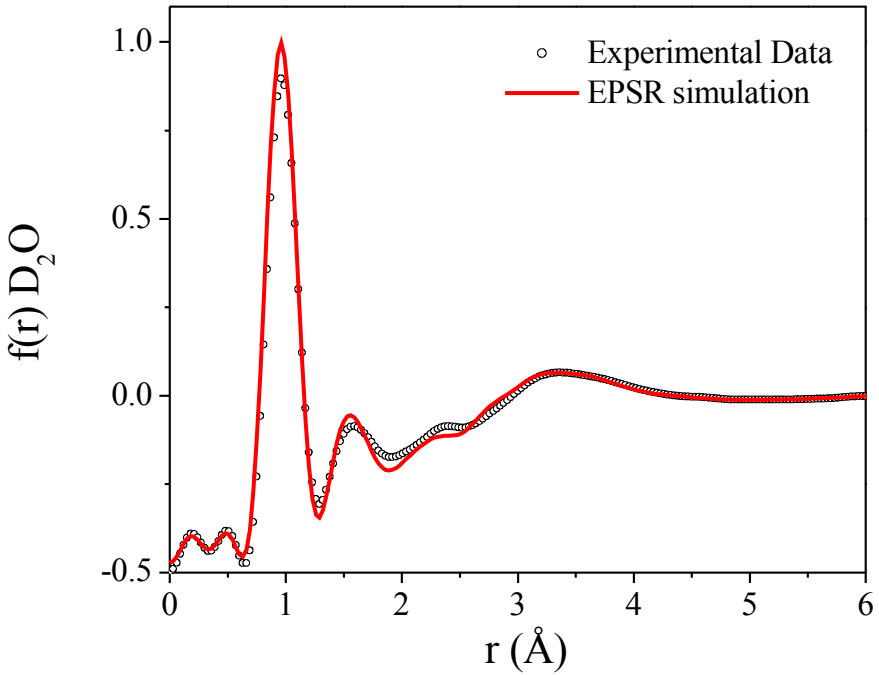
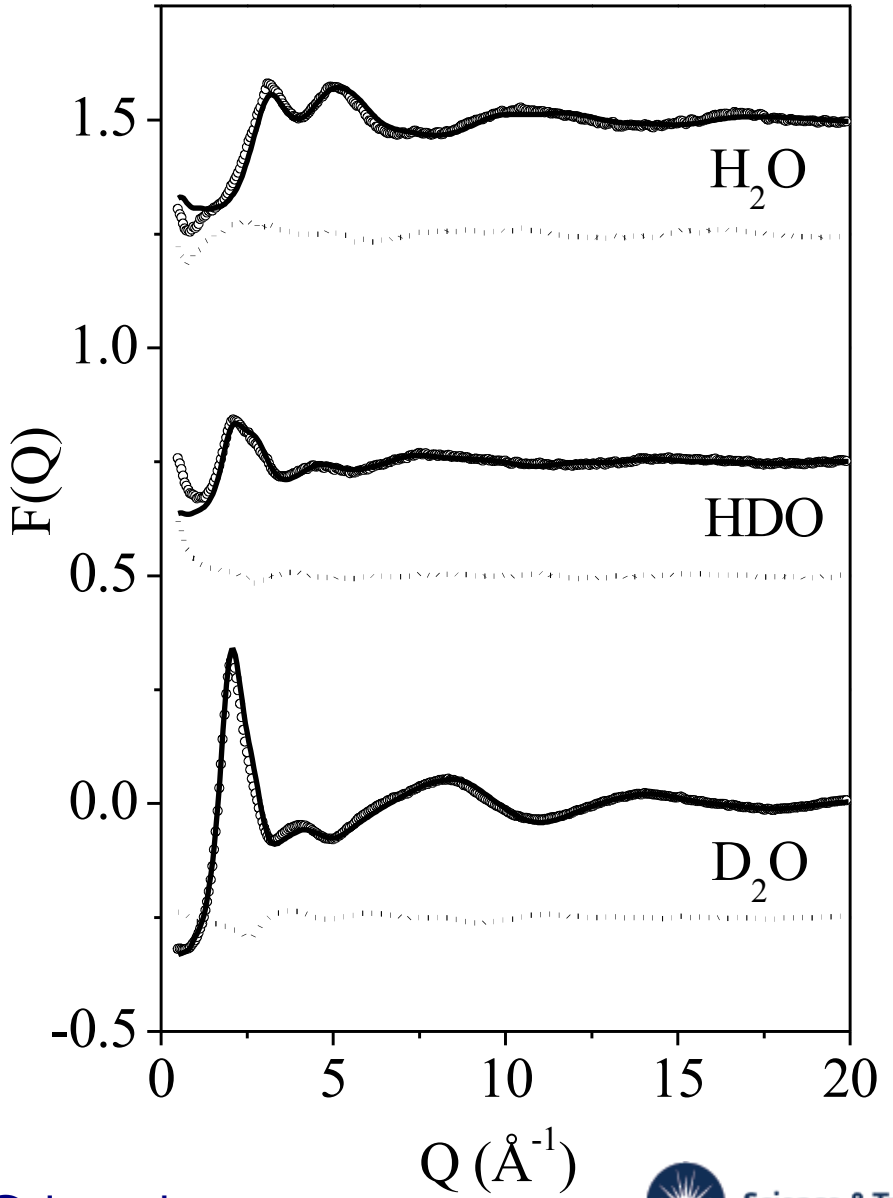
Experimental data and EPSR model for 1.0m YCl_3 in water





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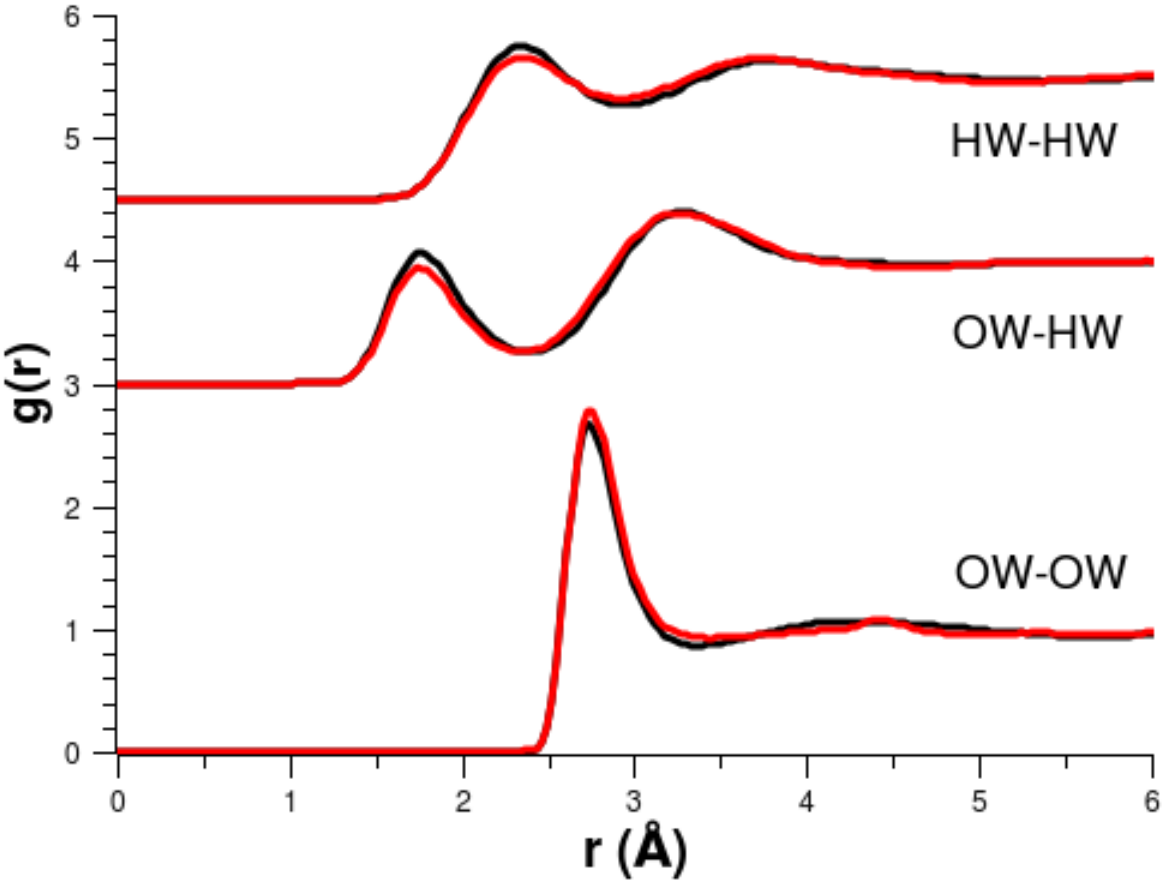
Water structure in a 1.0m YCl_3 solution

	Range Å	Pure Water	1m YCl_3 solution
OW-OW	2.3 - 3.3	4.3 ± 0.1	4.5 ± 0.1
OW-HW	1.4 - 2.5	2.0 ± 0.1	1.7 ± 0.1
HW-HW	1.5 - 3.0	5.6 ± 0.1	5.2 ± 0.1



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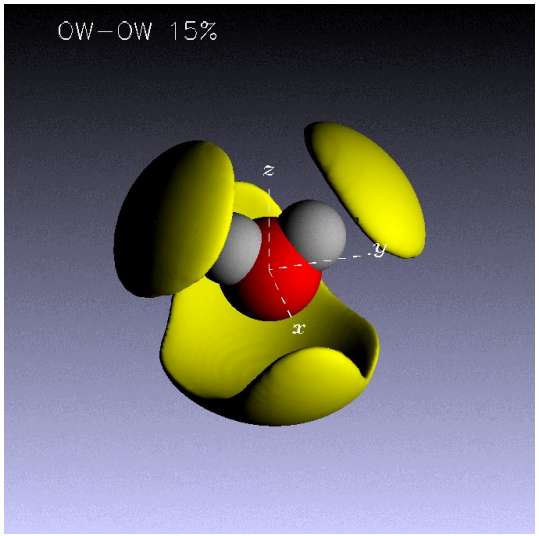
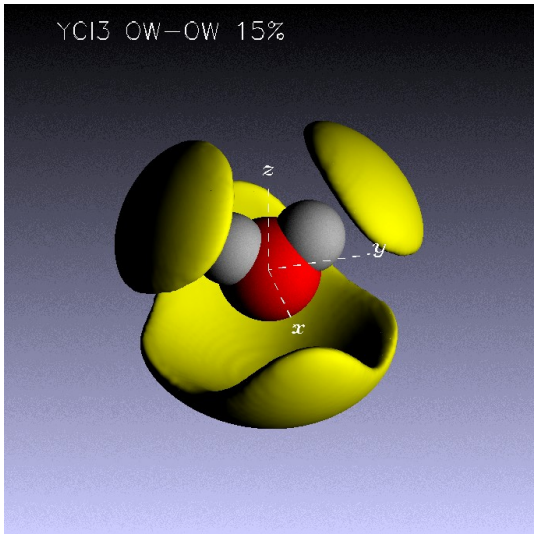
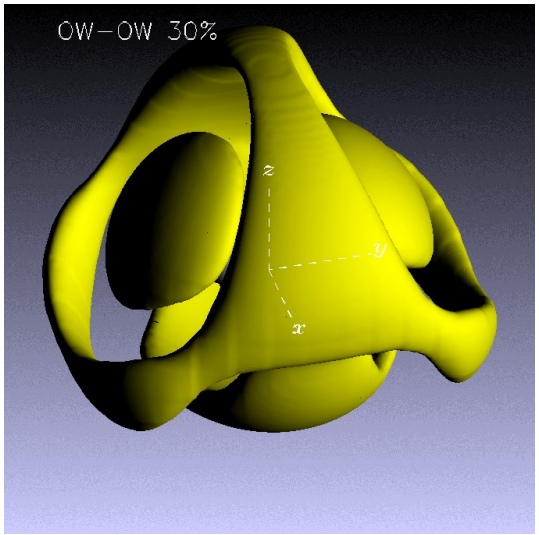
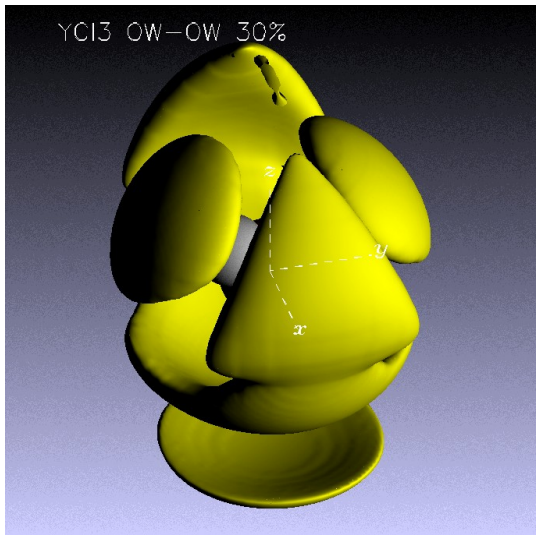
Change in water structure on addition of YCl_3

Water | **1.0m YCl_3**









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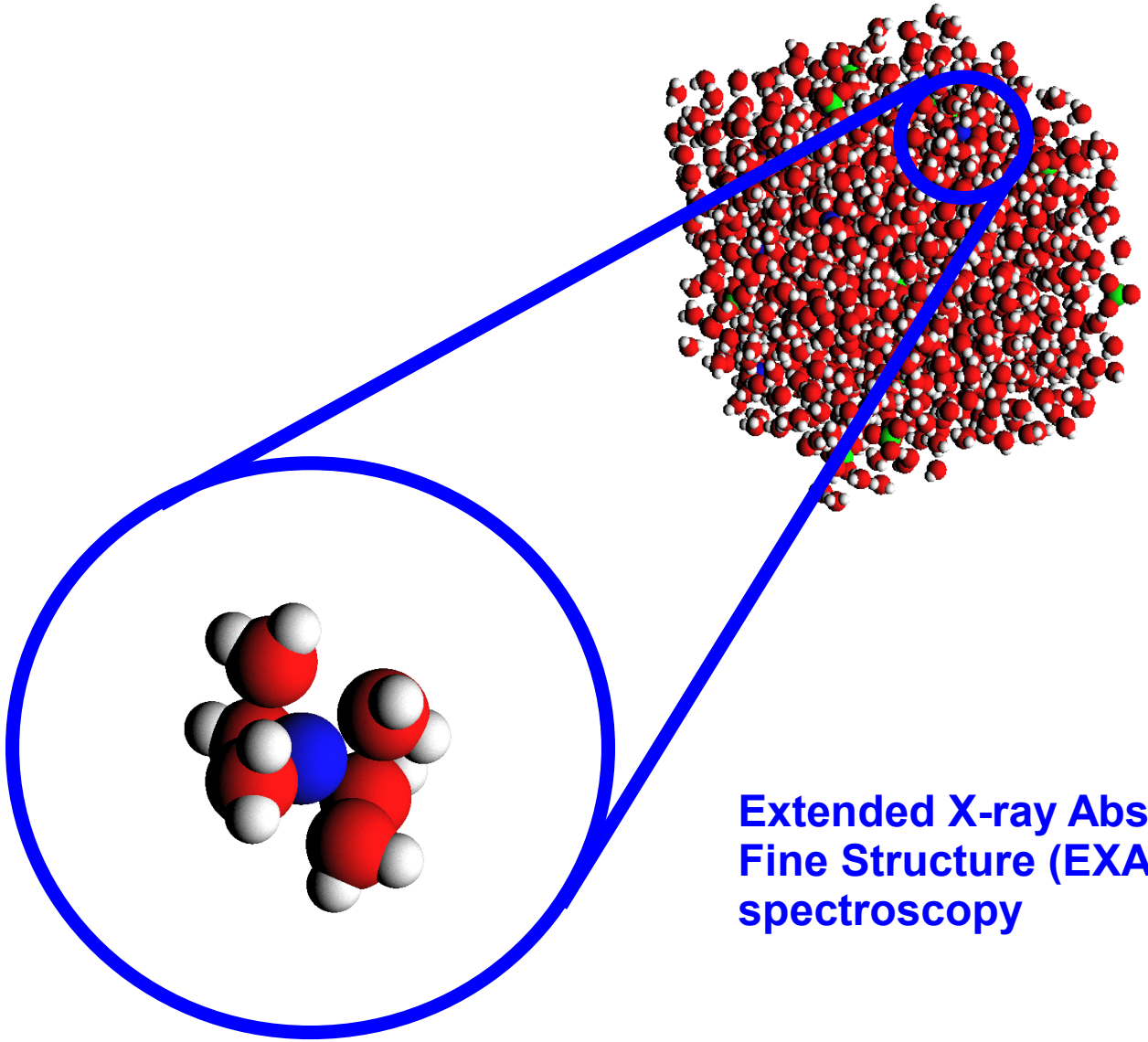
Step 2: Confirmation of the local structure by EXAFS spectroscopy



Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy

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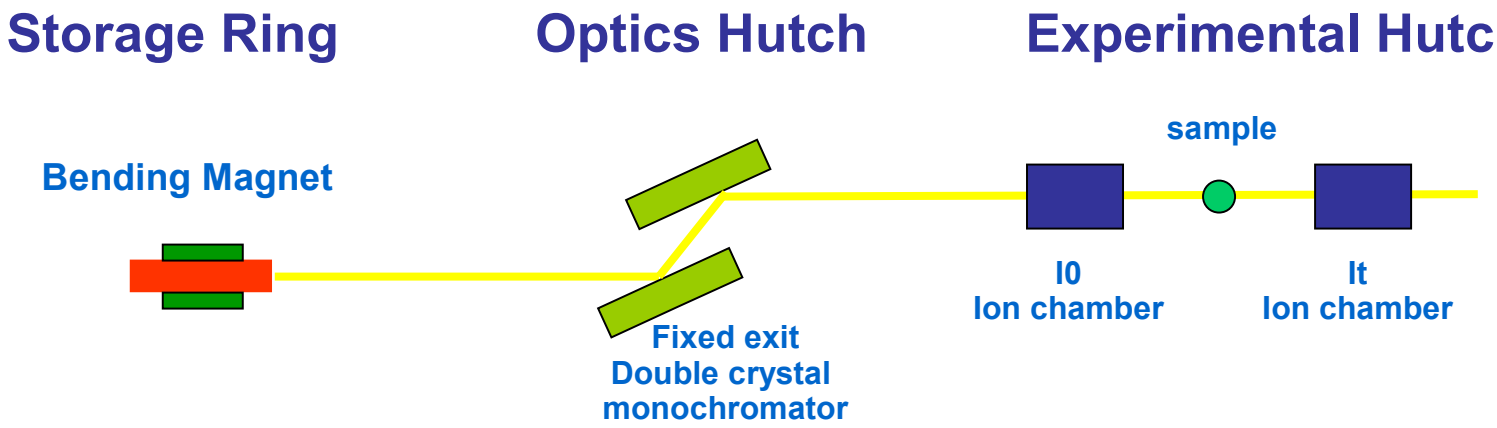
EXAFS measurements



$I_t = I_0 e^{-\mu(E)x}$

Where x: thickness of the sample

μ : absorption coefficient

EXAFS

$\mu(E)x = \ln(I_0/I_t)$

$\mu(E) = \mu_0(E)\{1 + \chi(k)\}$

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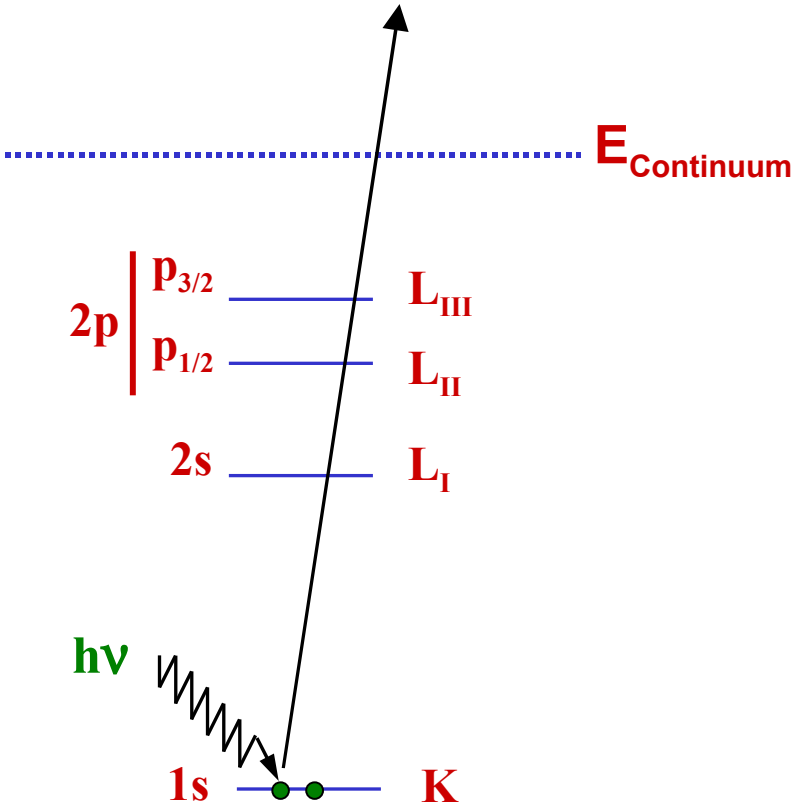
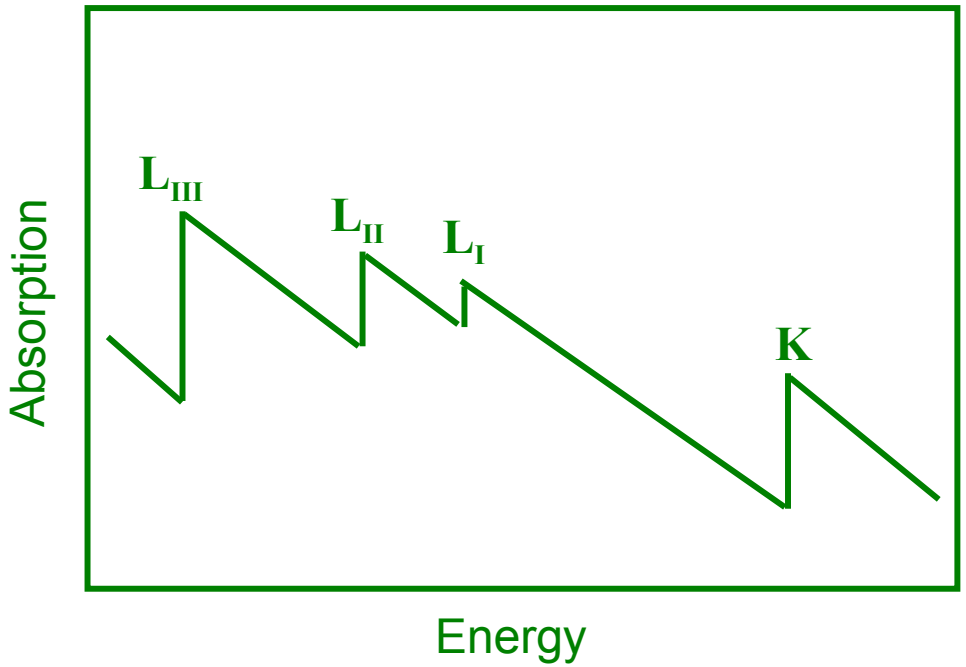
X-ray Absorption Spectroscopy





Permitted transitions → Selection rules → $\Delta l = \pm 1$

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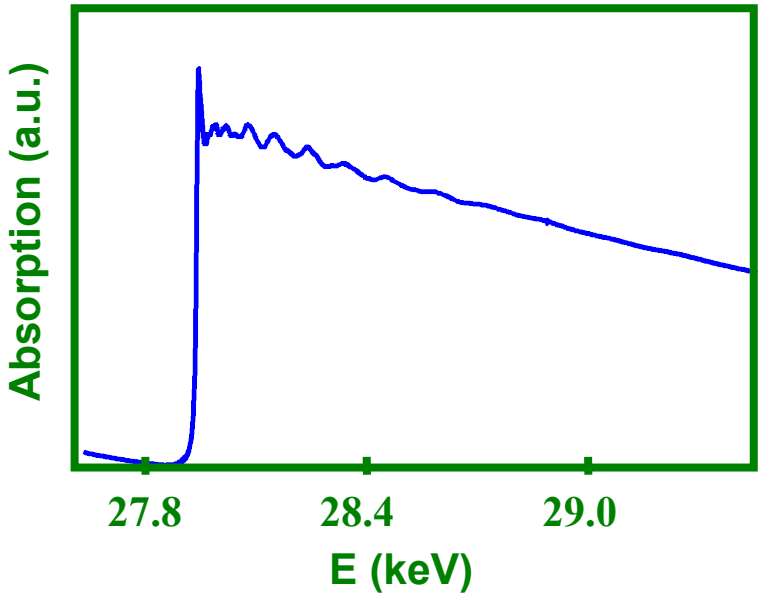
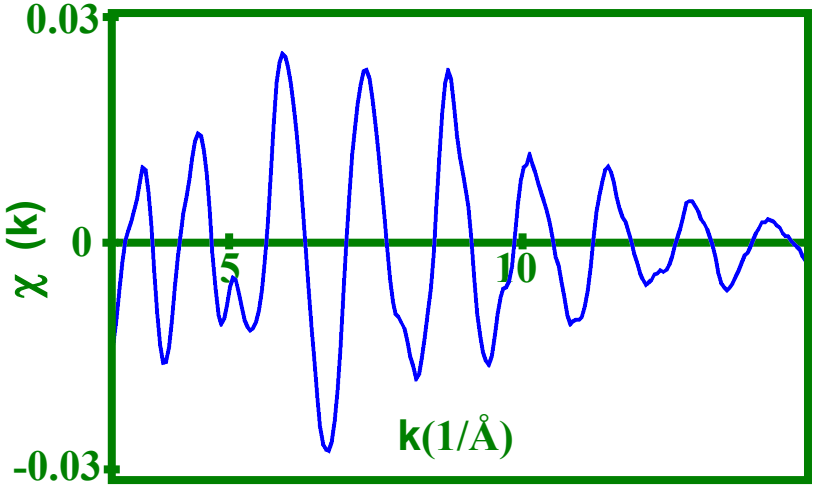
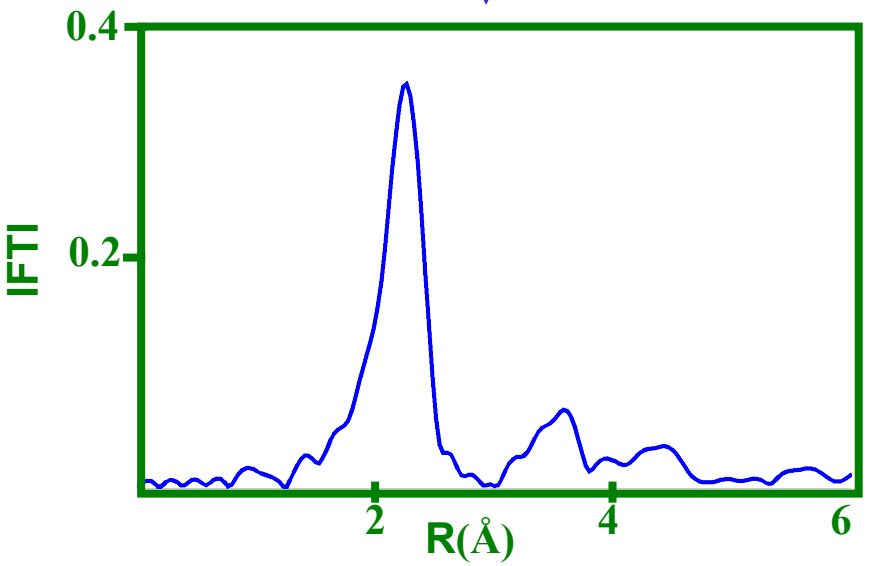
EXAFS





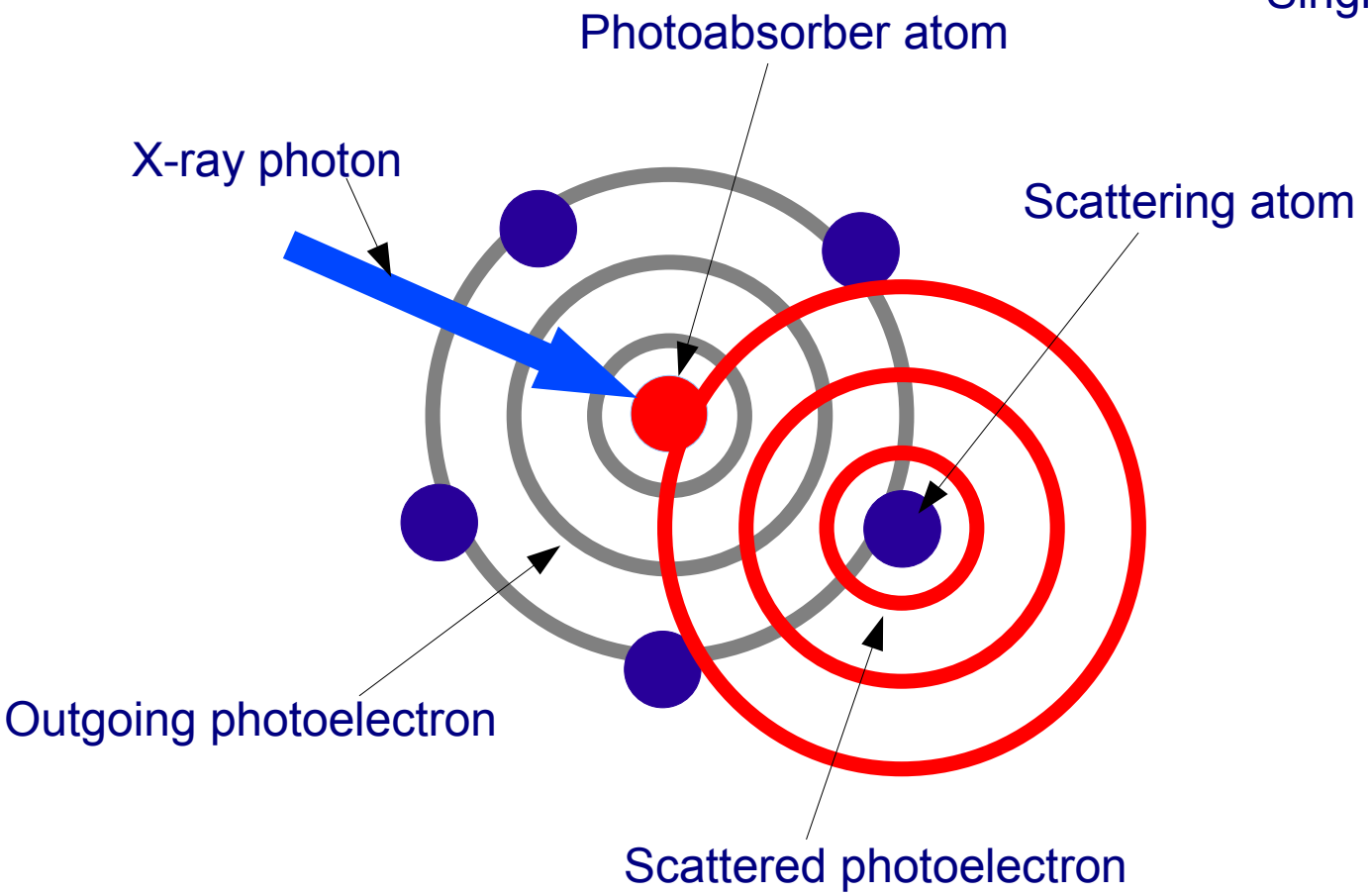


Information about:

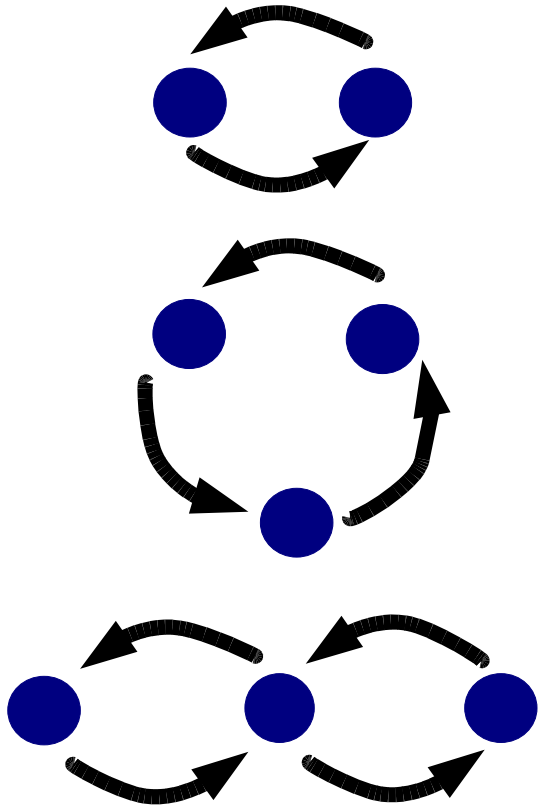
- Type of neighbors
- Number of neighbors
- Radial distribution around the absorbing atom
- Disorder.

EXAFS shell model

$$\chi(k) = \sum_R S_0^2 N_R \frac{|f(k)|}{\mathrm{kR}^2} \sin(2\mathrm{kR} + 2\delta_c + \Phi) e^{-2R/\lambda(k)} e^{-2\sigma^2 k^2}$$



Single and multiple scattering paths



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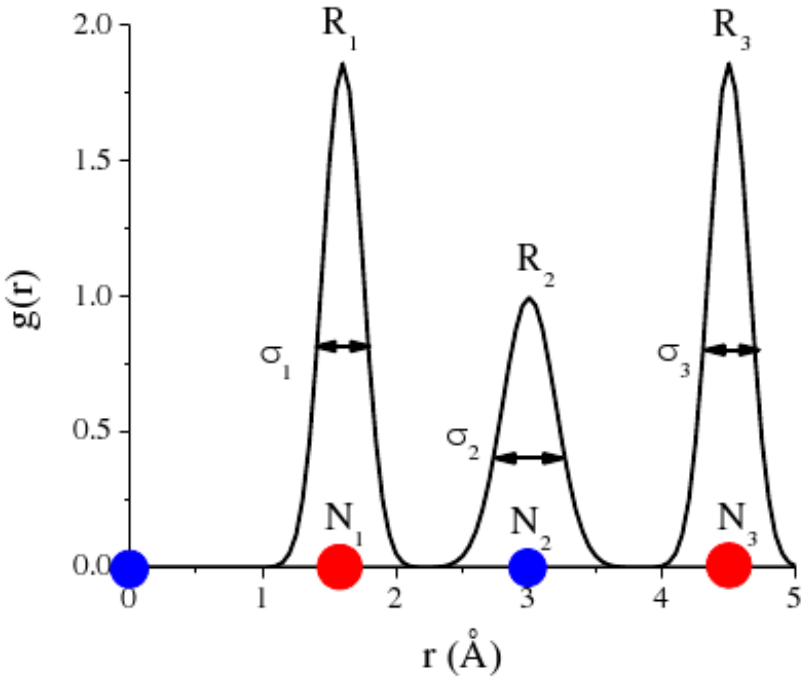
The Gaussian shell model for EXAFS analysis

$$\chi(k) = \sum_j \frac{N_j}{kR_j^2} e^{2R_j/\lambda_j(k)} \left| f_j(k,\pi) \right| \sin\left(2kR_j + 2\delta_l'(k) + \phi_j(k)\right) e^{-2\sigma_j^2 k^2}$$



R_j = Distance of photo-absorber to shell j
N_j = Number of atoms in shell j
$\exp(-2\sigma^2_j k^2)$ = Debye-Waller disorder for shell j
$|f_j(k,\pi)|$ = Backscattering amplitude of shell j
$\phi_j(k)$ = Backscattering phase function of shell j
$\delta_l'(k)$ = Photo-absorber phase function
λ_j = Mean-free path term for inelastic losses

Works well for crystalline solids and well defined molecular structures

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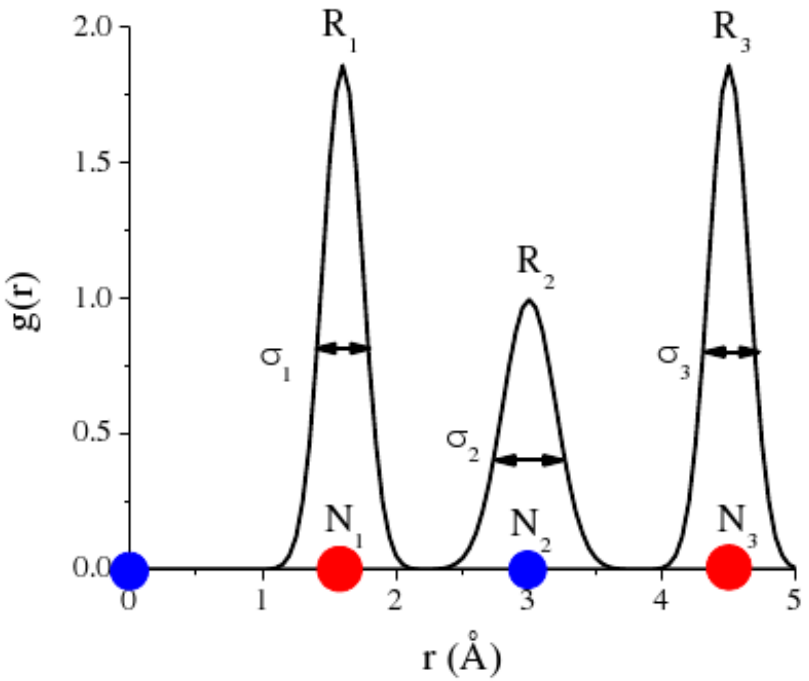
The Gaussian shell model for EXAFS analysis

$$\chi(k) = \sum_j \frac{N_j}{kR_j^2} e^{2R_j/\lambda_j(k)} \left| f_j(k,\pi) \right| \sin\left(2kR_j + 2\delta_l'(k) + \phi_j(k)\right) e^{-2\sigma_j^2 k^2}$$

Convenient for peak fitting analysis based on a (significant) number of free parameters



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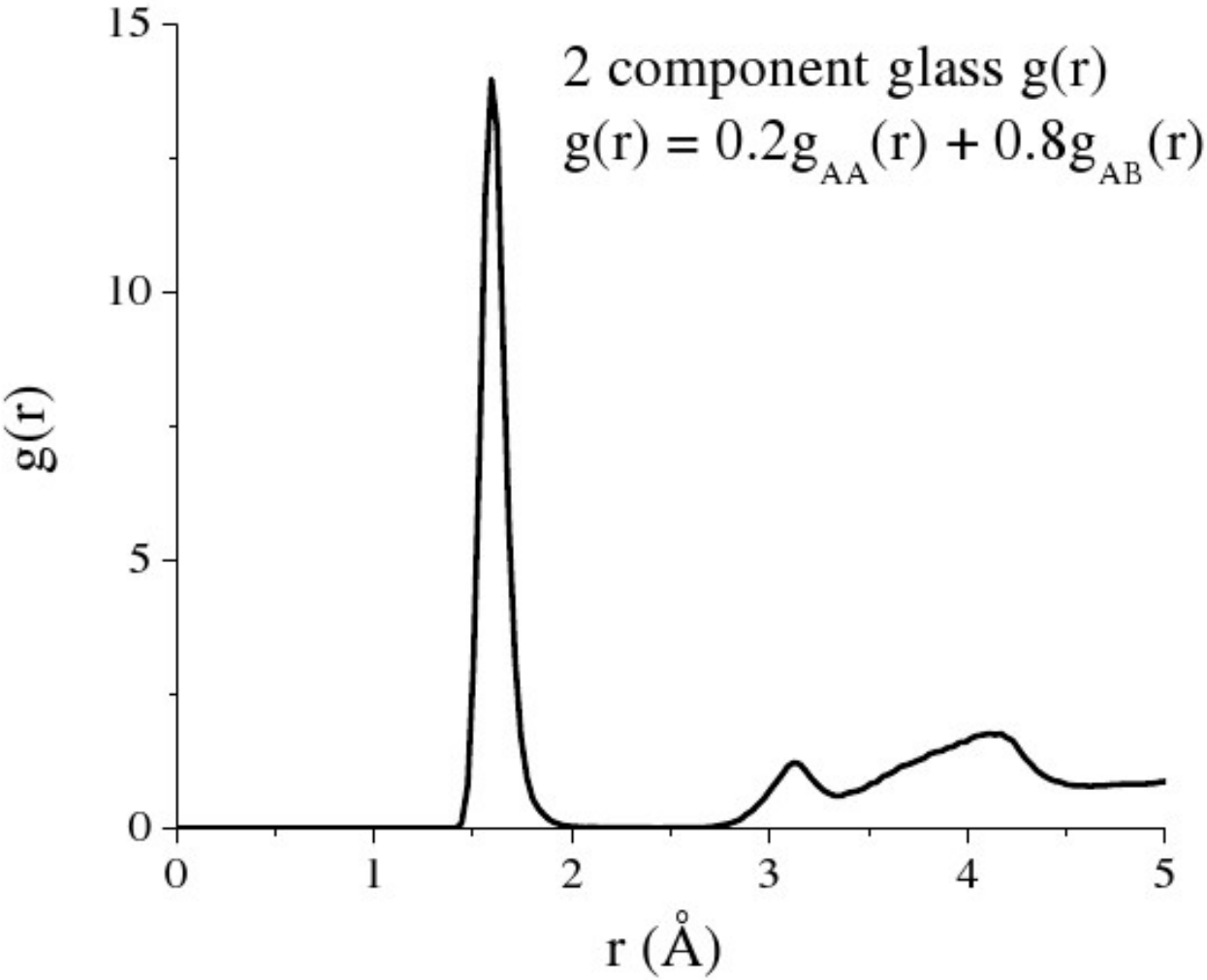
Breakdown of the EXAFS shell model

Liquids and disordered materials are best characterised by the radial distribution function g(r)



Breakdown of the EXAFS shell model

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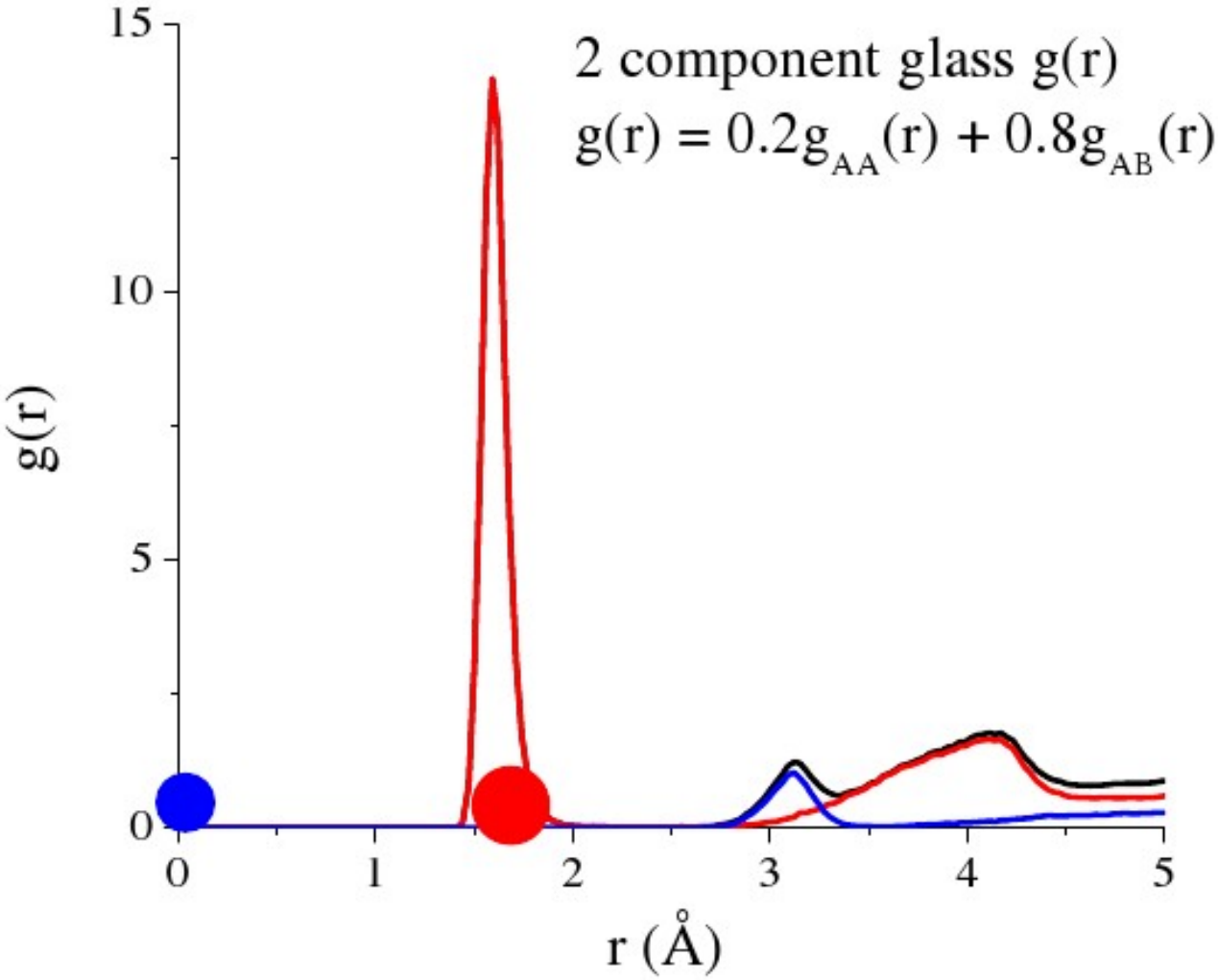

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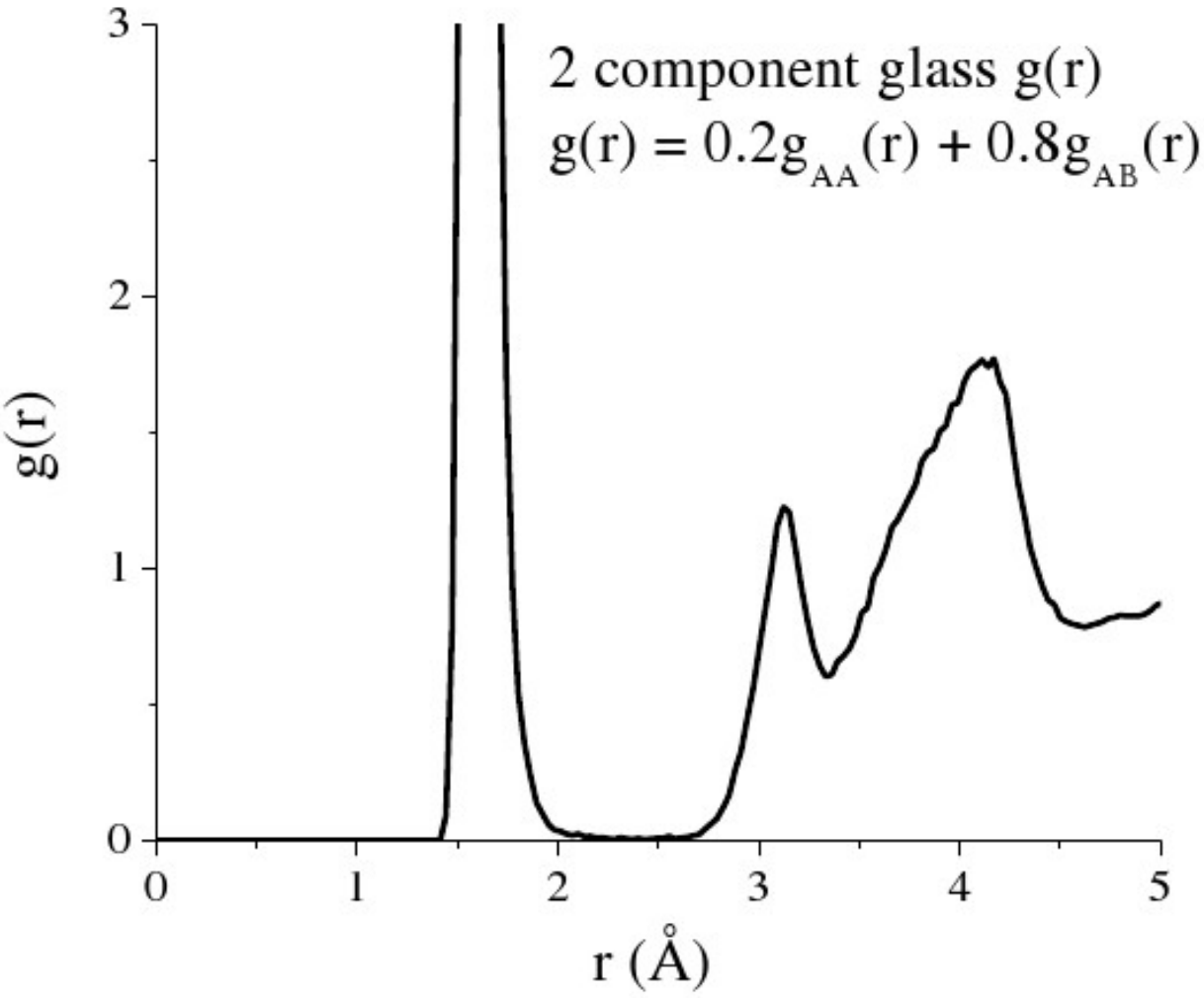

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Breakdown of the EXAFS shell model

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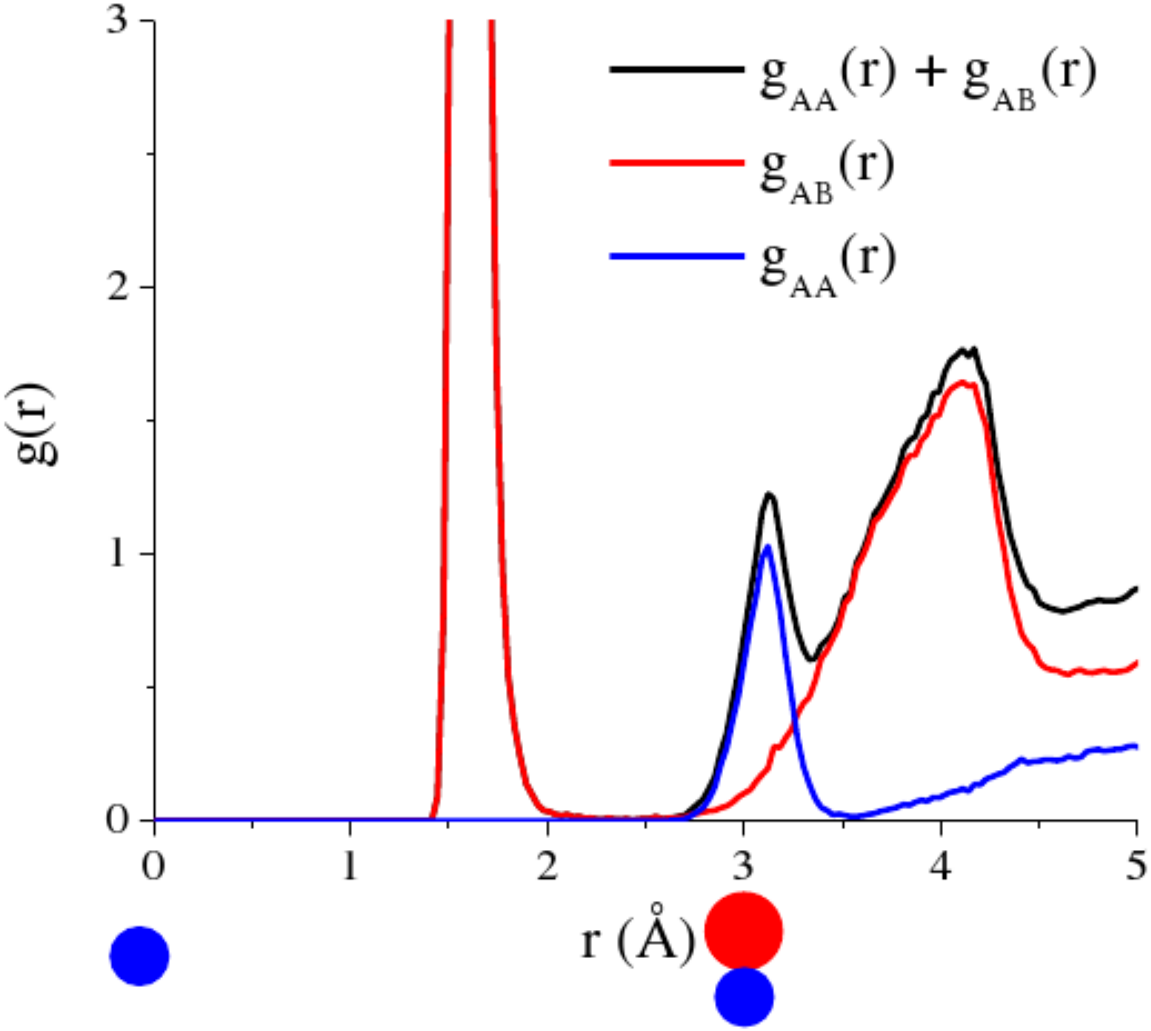

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Reformulation of the EXAFS equation as a configurational average

$$\chi(k) = \sum_i \gamma^{(2)}(0,i)$$

$\gamma^{(2)}$ is the EXAFS signal associated with a single neighbour atom at a distance r from the photo-absorber.

$$\langle \chi(k) \rangle = \int_0^\infty dr 4\pi r^2 \rho g(r) \gamma^{(2)}(r,k)$$

$\langle \chi(\mathrm{k}) \rangle$ is the ensemble average of the pair-wise atomic configurations characterised by the radial pair distribution function, g(r), centred on the photo-absorber. This function intrinsically incorporates the static and dynamic disorder in the local environment.

A.Filipponi, *J. Phys. Condens. Matter*, **13**, R23 (2001)

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Reformulation of the EXAFS equation

$$\langle \chi(k) \rangle = \int_0^\infty dr 4\pi r^2 \rho g(r) \gamma^{(2)}(r,k)$$

$\gamma^{(2)}$ contains the chemically specific phase and backscattering amplitude information

Phase term

$$\gamma^{(2)}(r,k) = A(k,r)\sin(2kr + \phi(k,r))$$

Atom, energy and distance dependent loss term

Backscattering amplitude

$$A(k,r) = \frac{f(k,r)}{kr^2}\exp(-r/\lambda(k,r))$$

A.Filipponi, *J. Phys. Condens. Matter*, **6**, 8415 (1994)

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Complementarity between Diffraction and EXAFS

A diffraction experiment probes the pair correlation function g(r):

$$S(Q)=1+\frac{4\pi\rho}{Q}\int_0^\infty (g_2(r)-1)r\sin(\mathrm{Qr})\,\mathrm{dr}$$

For a fixed atom configuration around a photoabsorber, the EXAFS can be written as:

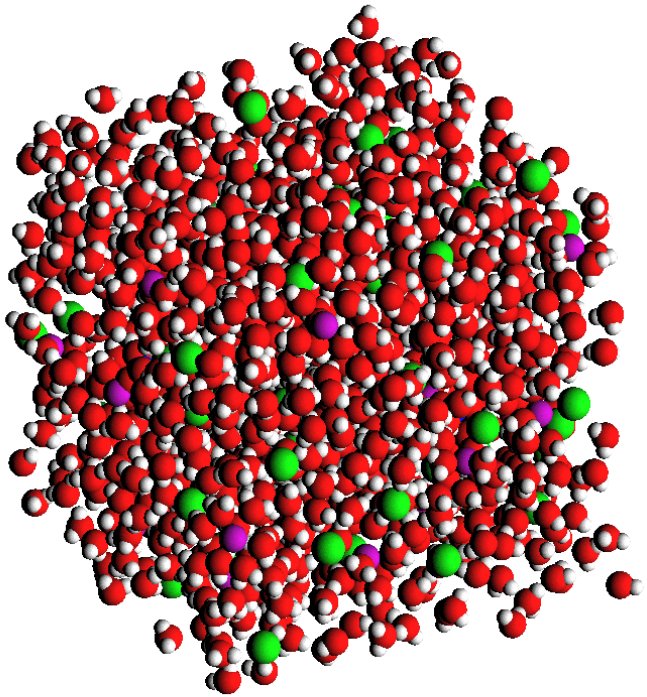
$$\chi(k)=\sum_i \gamma^{(2)}(0,i)+\sum_{(i,j)} \gamma^{(3)}(0,i,j)+\ldots$$

To apply this to a real system we need to ensemble average to include structural and dynamic disorder. This is achieved through the inclusion of the pair and higher order correlation functions:

$$\langle\chi(k)\rangle=\int_0^\infty \mathrm{dr}\,4\pi r^2\rho g(r)\gamma^{(2)}(r,k)+\int \mathrm{dr}_1\,\mathrm{dr}_2\,d\phi\,8\pi^2 r_1^2 r_2^2\sin(\phi)\rho^2 g_3(r_1,r_2,\phi)\gamma^{(3)}(r_1,r_2,\phi,k)$$

A.Filipponi, *J. Phys. Condens. Matter*, **13**, R23 (2001)

EXAFS from an EPSR model



Step 1: select a photoabsorbing atom within the simulation box and place at origin

Step 2: identify neighbouring atom coordinates within a radius of 6Å (cluster for potential, phase shift and scattering path calculations)

Step 3: Calculate theoretical EXAFS signal using no Debye-waller broadening (e.g. FEFF 8) and all significant paths

Step 4: repeat for all photoabsorbing atoms in the box, and average signals

Step 5: continue simulation and repeat process for many boxes

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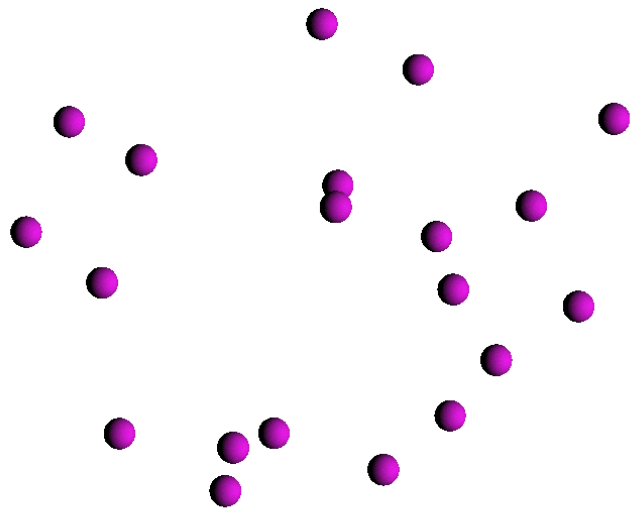
EXAFS from an EPSR model



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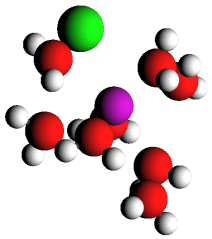
EXAFS from an EPSR model



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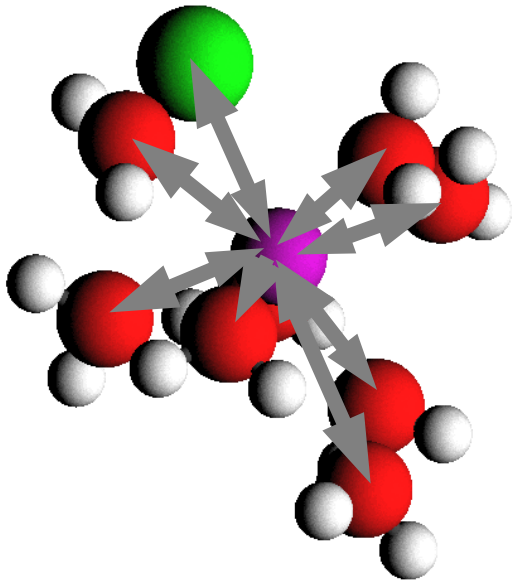
EXAFS from an EPSR model



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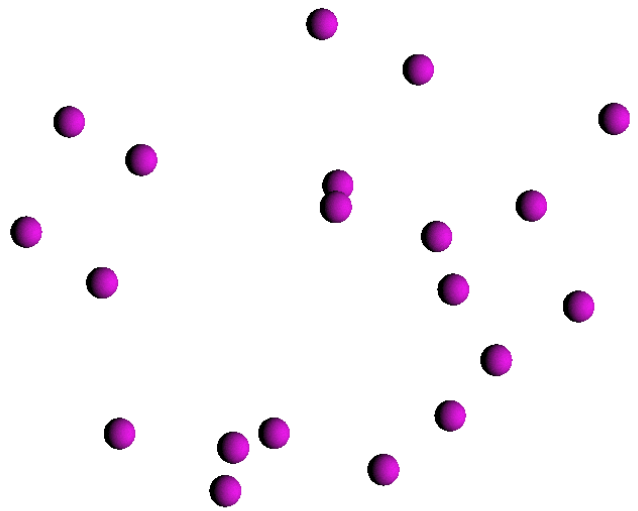

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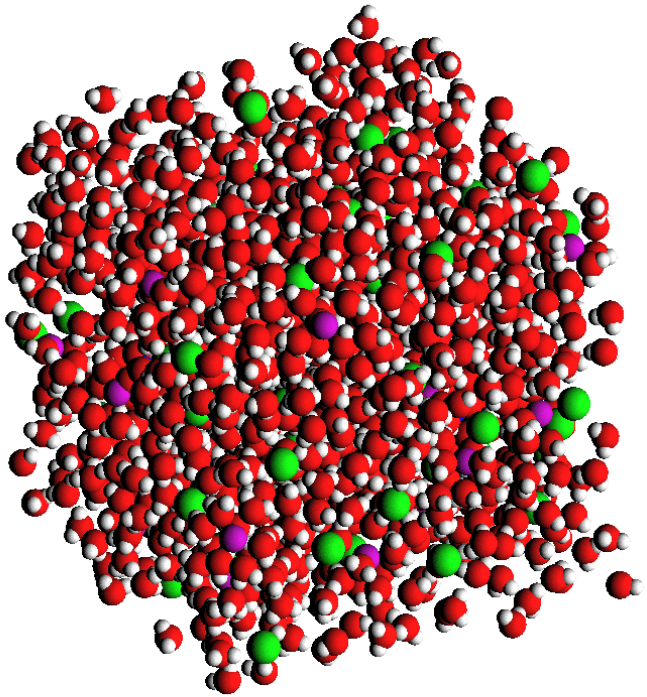
EXAFS from an EPSR model



Hundreds to thousands of configurations are generally required to correctly account for the continuous nature of the radial distribution function and to ensure stability of the final local structure model.

Step 1: select a photoabsorbing atom within the simulation box and place at origin

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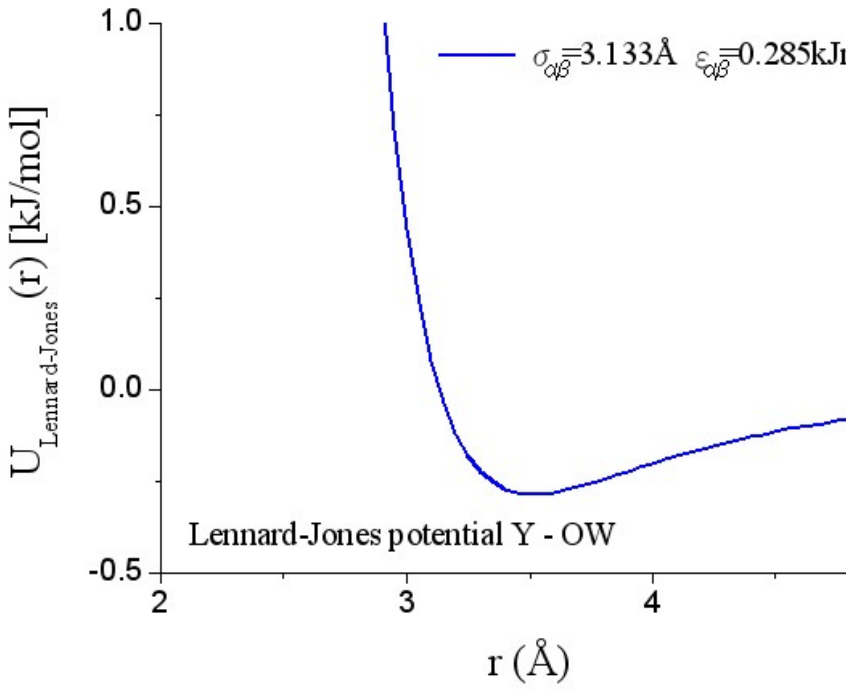
Step 4: repeat for all photoabsorbing atoms in the box, and average signals

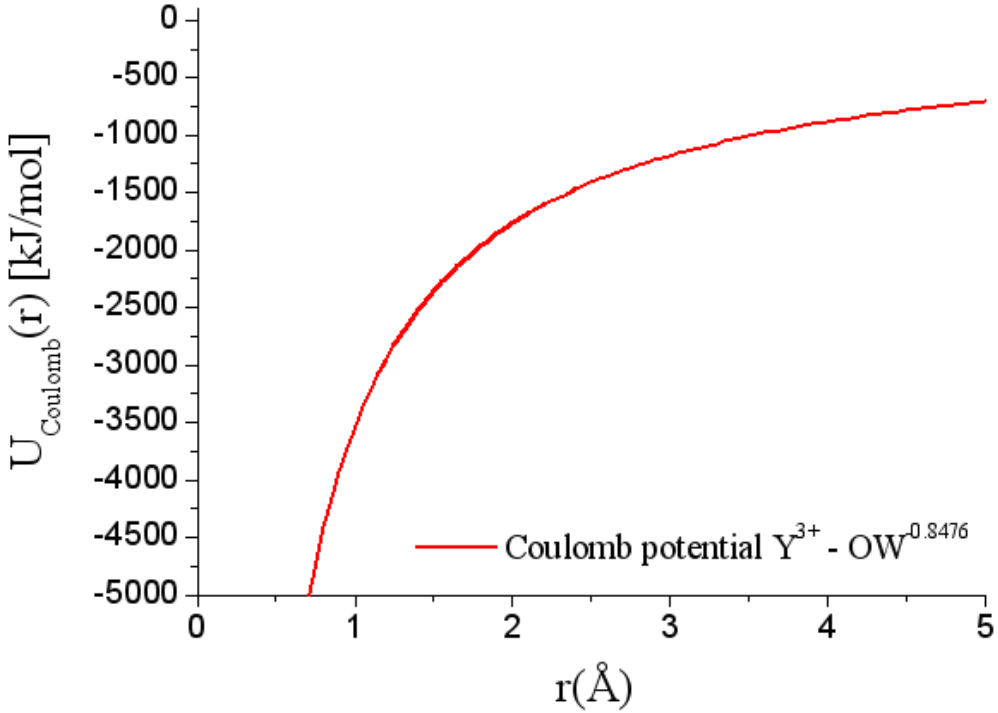
Step 5: continue simulation and repeat process for many boxes

Y^{3+}-OW interaction potential used in the structure refinement

$$U_{\alpha\beta}(r) = 4\varepsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r_{ij}}\right)^{6}\right] + \frac{q_\alpha q_\beta}{4\pi\varepsilon_0 r_{ij}}$$

$$\varepsilon_{\alpha\beta} = \left(\varepsilon_\alpha \varepsilon_\beta\right)^{\frac{1}{2}} \qquad \sigma_{\alpha\beta} = \frac{1}{2}\left(\sigma_\alpha + \sigma_\beta\right)$$





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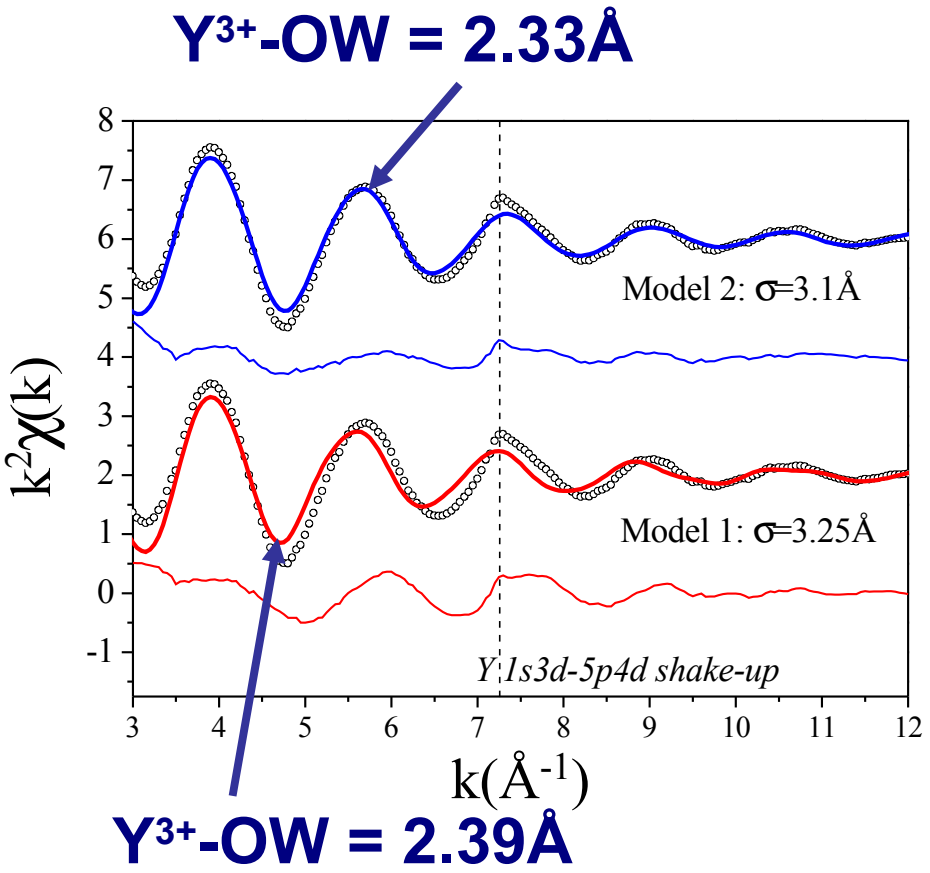
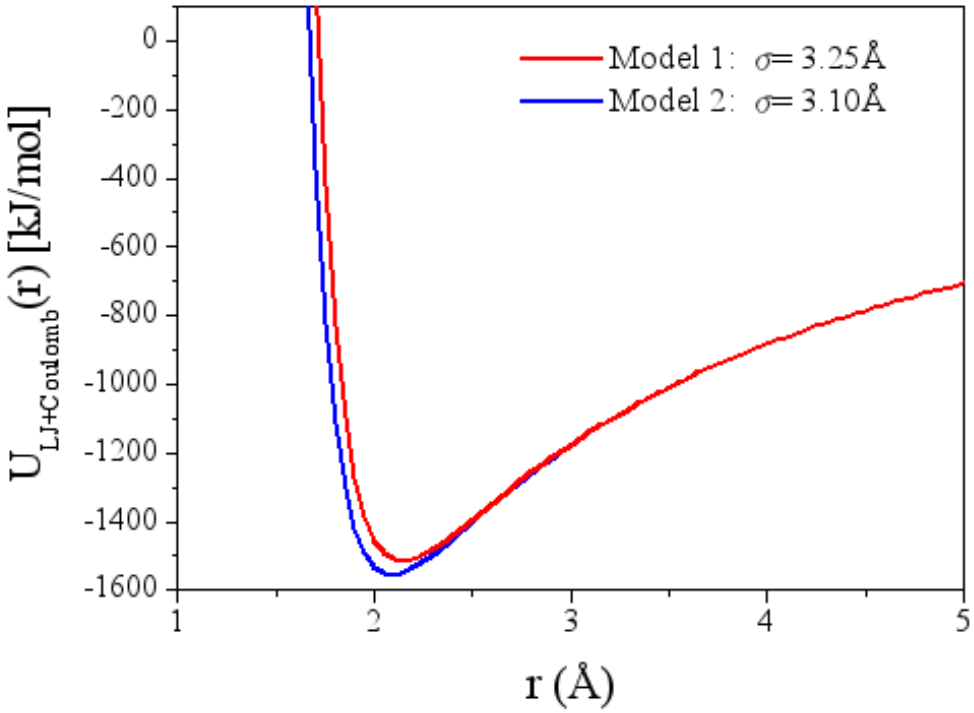
Sensitivity of the EXAFS model to the choice of reference potential





D.T.Bowron and S.Díaz-Moreno *J. Phys. Chem. B*, **111** 11393 (2007)

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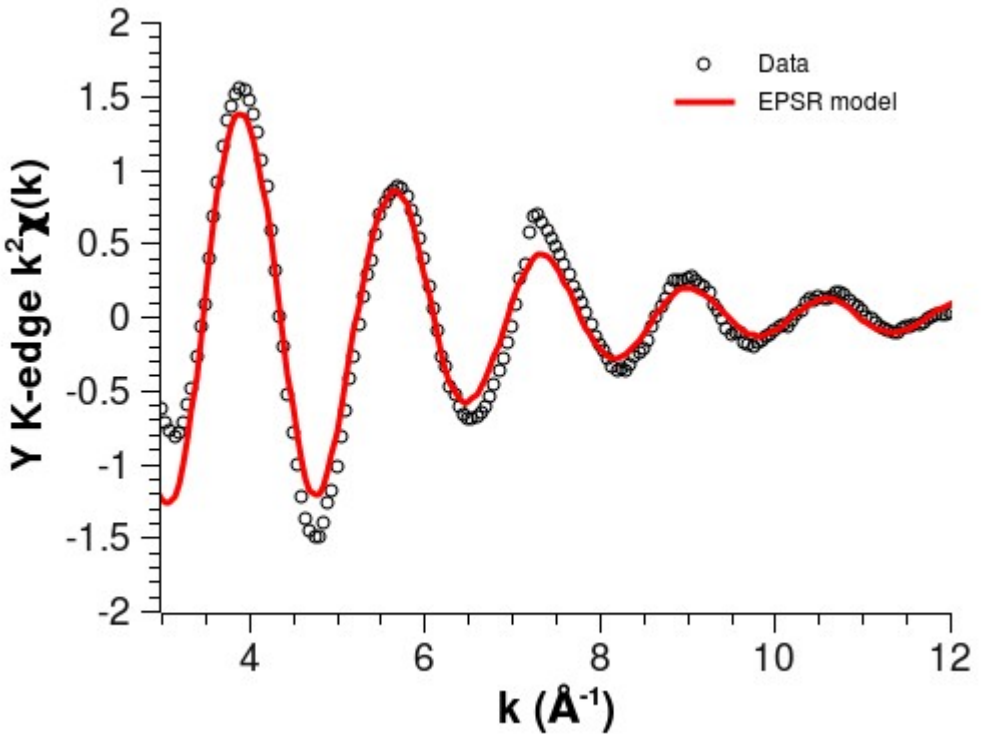
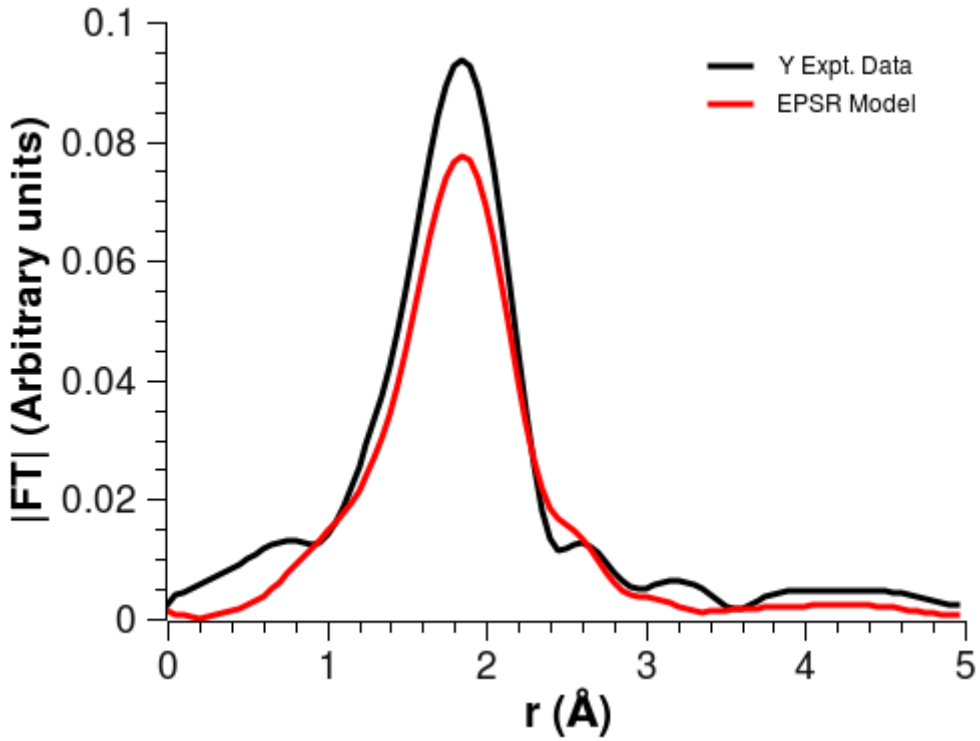
EPSR prediction for the Y K-edge EXAFS signal in 1.0m YCl_3 solution





Experimental data taken from: S.Diaz-moreno, A.Muñoz-Páez, J.Chaboy
J. Phys. Chem. A **104** 1278 (2000)
(1.0M solution)

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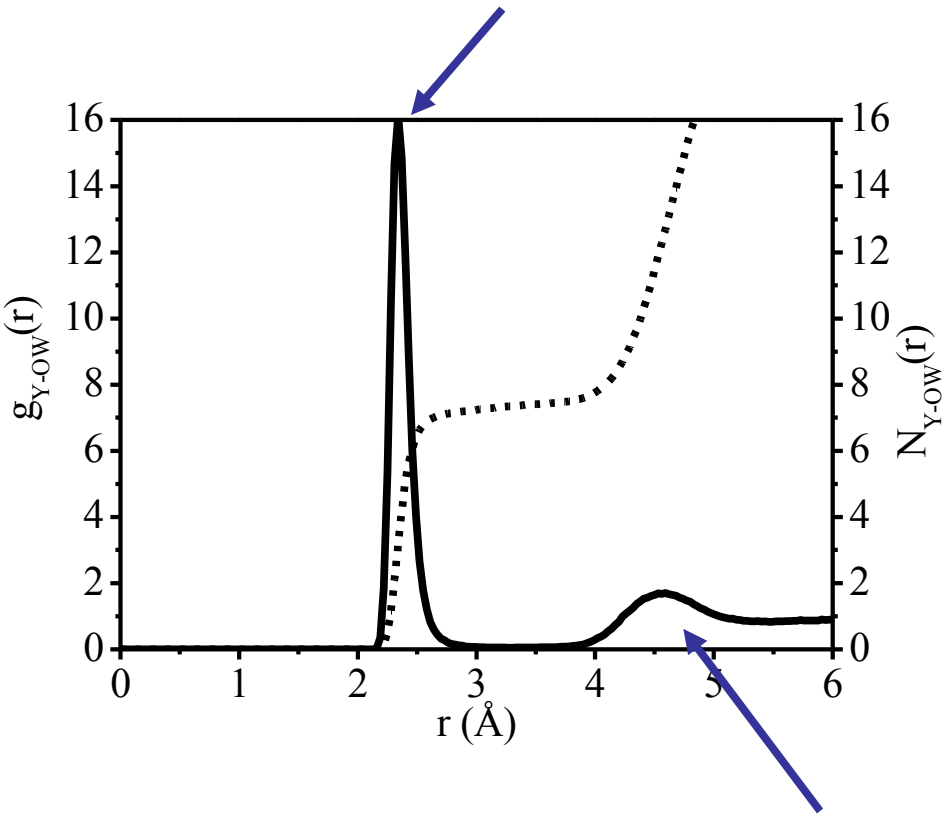
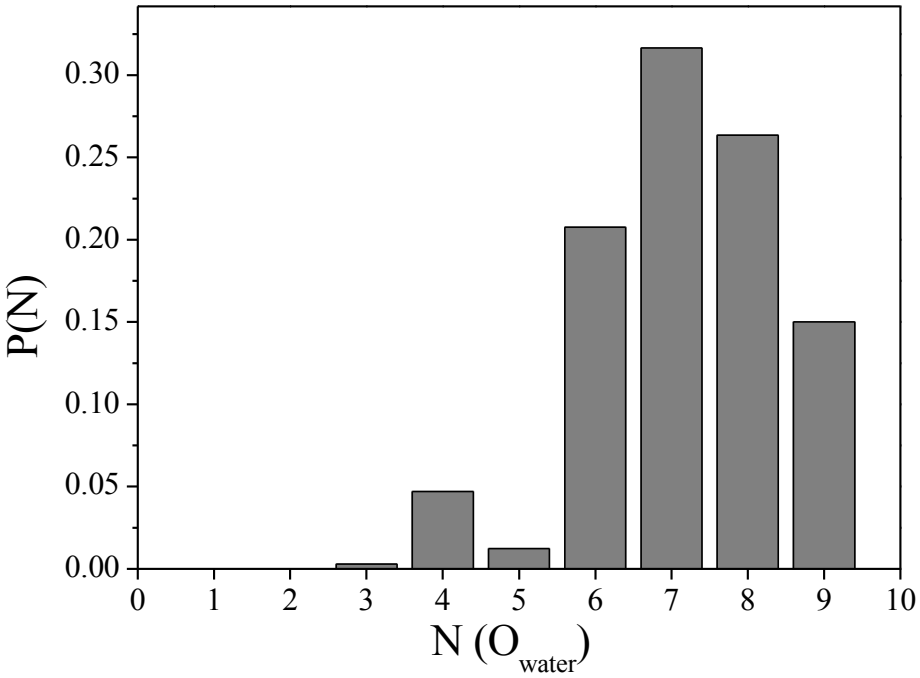
Y^{3+} hydration in a 1.0m YCl_3 solution: $g_{Y\text{-}OW}(r)$

Y^{3+}-OW = 2.33Å

Y^{3+}-OW mean C.N. 7.4±0.5





Well defined second hydration shell at ~ 4.6Å

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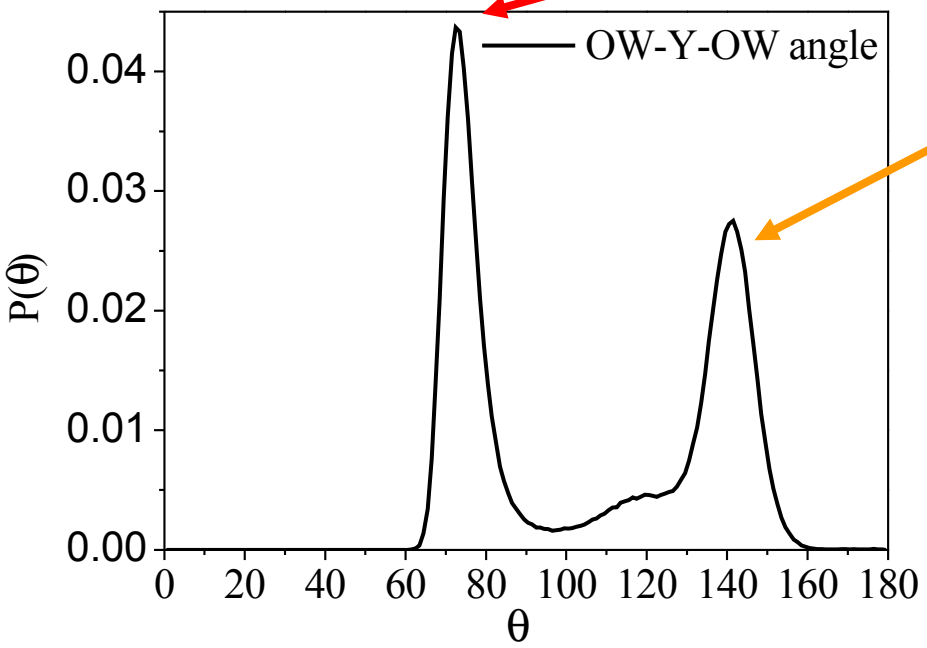
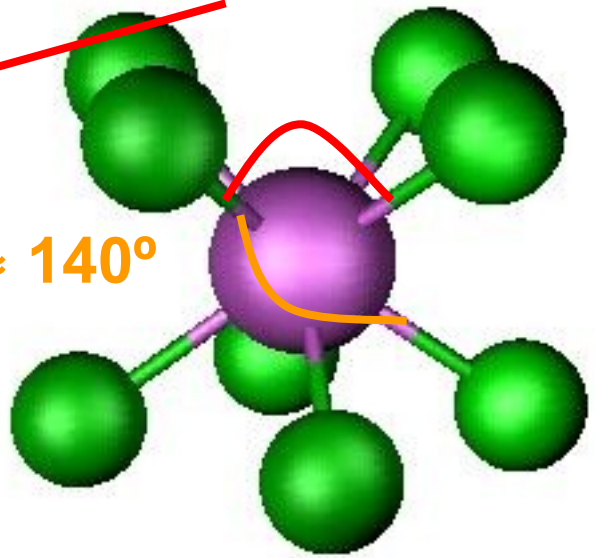
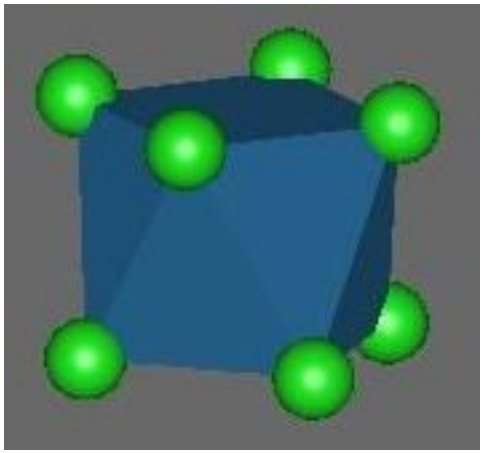
Local geometry of the Y^{3+} hydration shell



≈ 70°

≈ 140°





Square antiprism

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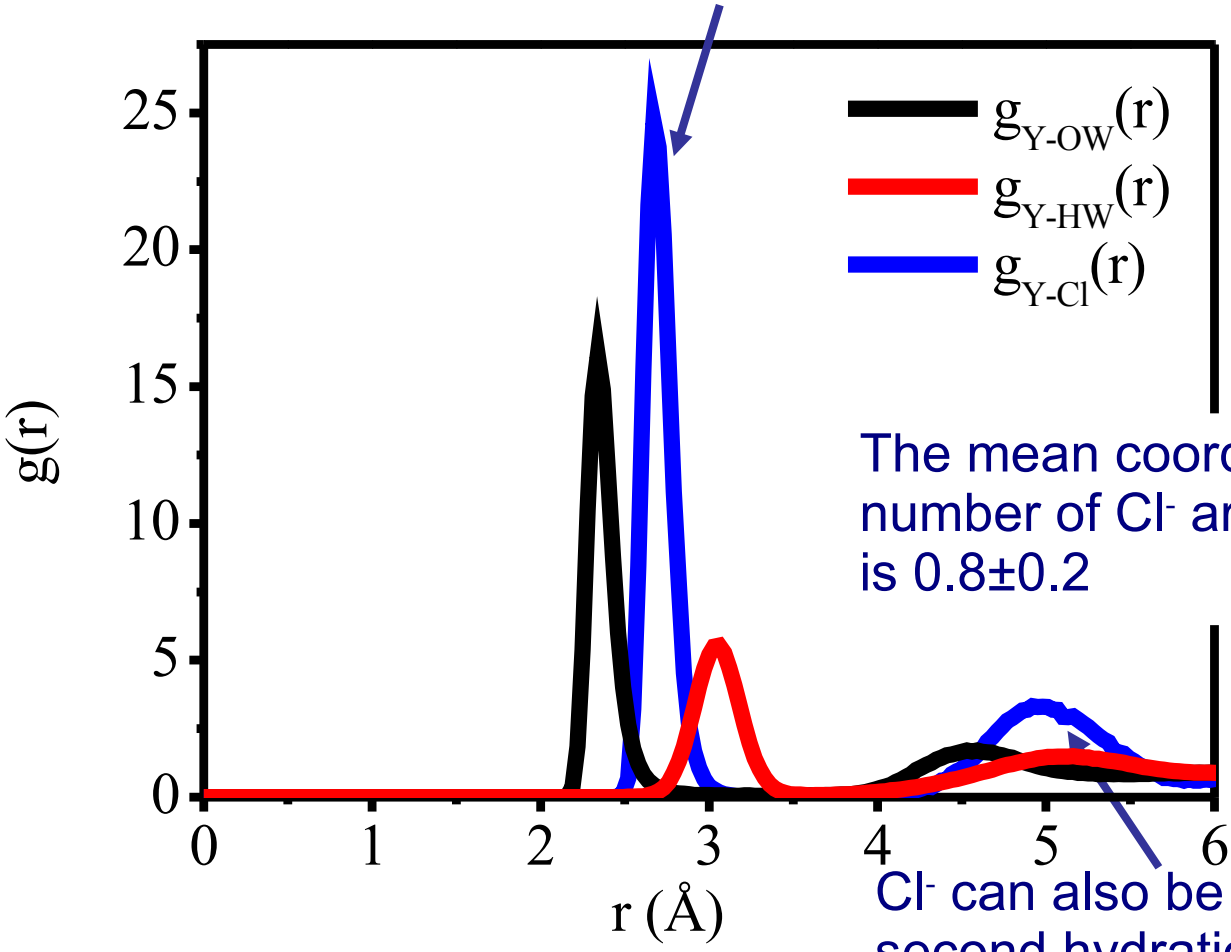
Ion-ion interactions in the Y^{3+} hydration shell

The model tells us that Cl^- anions can be found in the first hydration shell



The mean coordination number of Cl^- around Y^{3+} is 0.8±0.2

Cl^- can also be found in the second hydration shell of Y^{3+}

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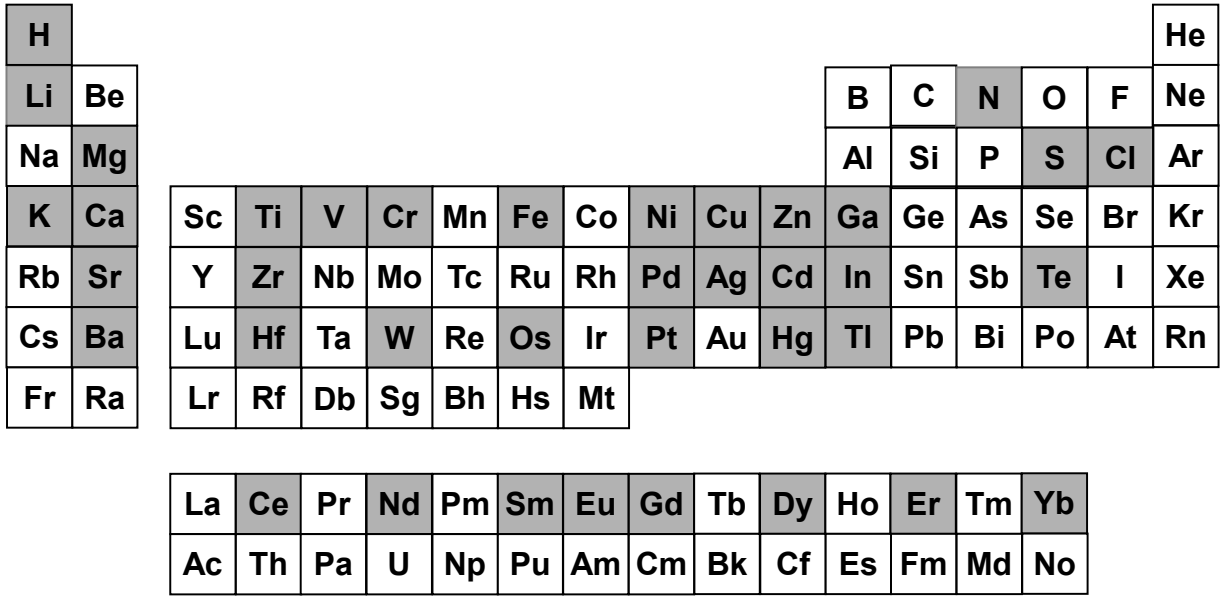
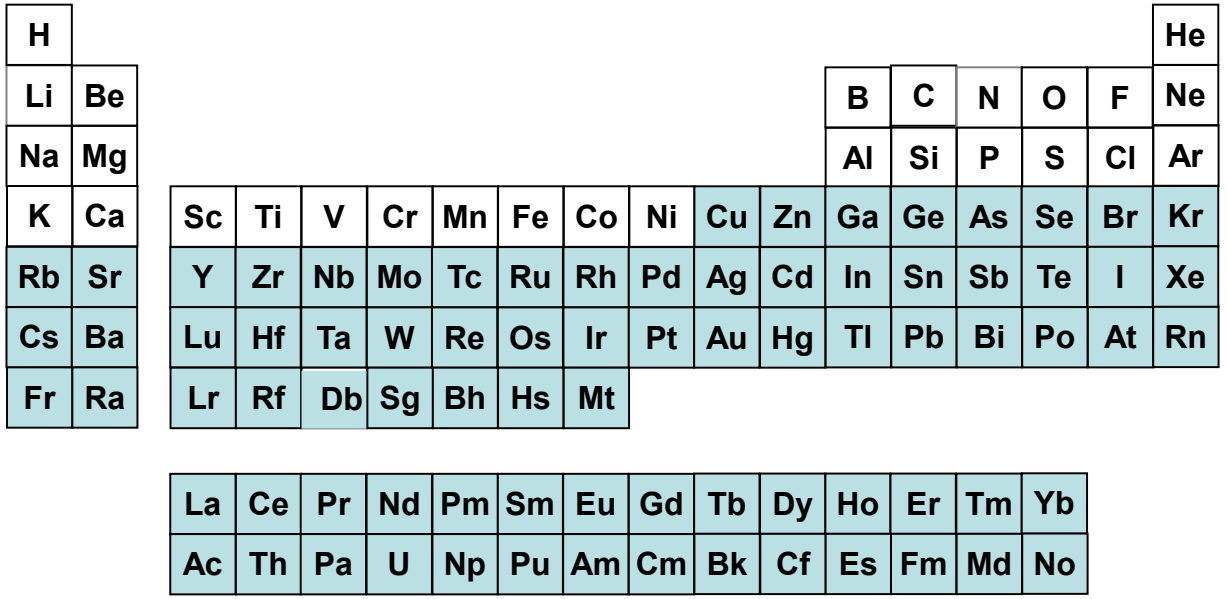
Isotopes and absorption edges – routes to chemical specificity



Elements with isotopes that potentially can be used for NDIS ion solvation studies ($\Delta\ b_c \geq\ 1$fm)

J.E.Enderby, *Chem. Soc. Revs.* 159 (1995)

Isotopes and absorption edges – routes to chemical specificity



Elements with absorption edges suitable for atomic resolution Anomalous X-ray Scattering investigation of local structure in solutions

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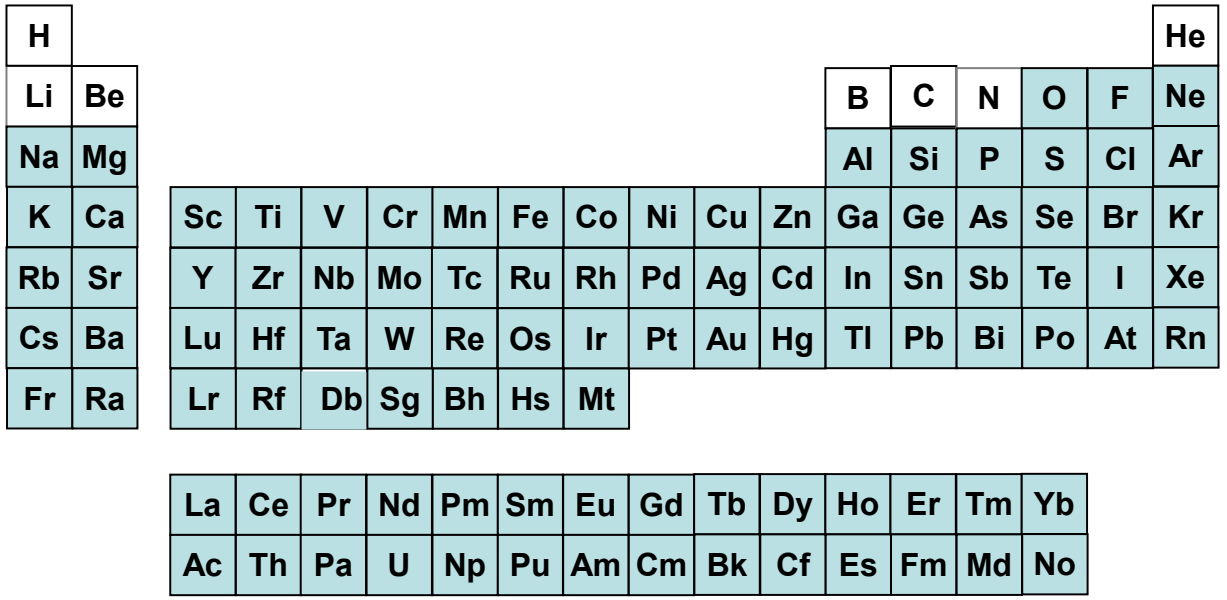
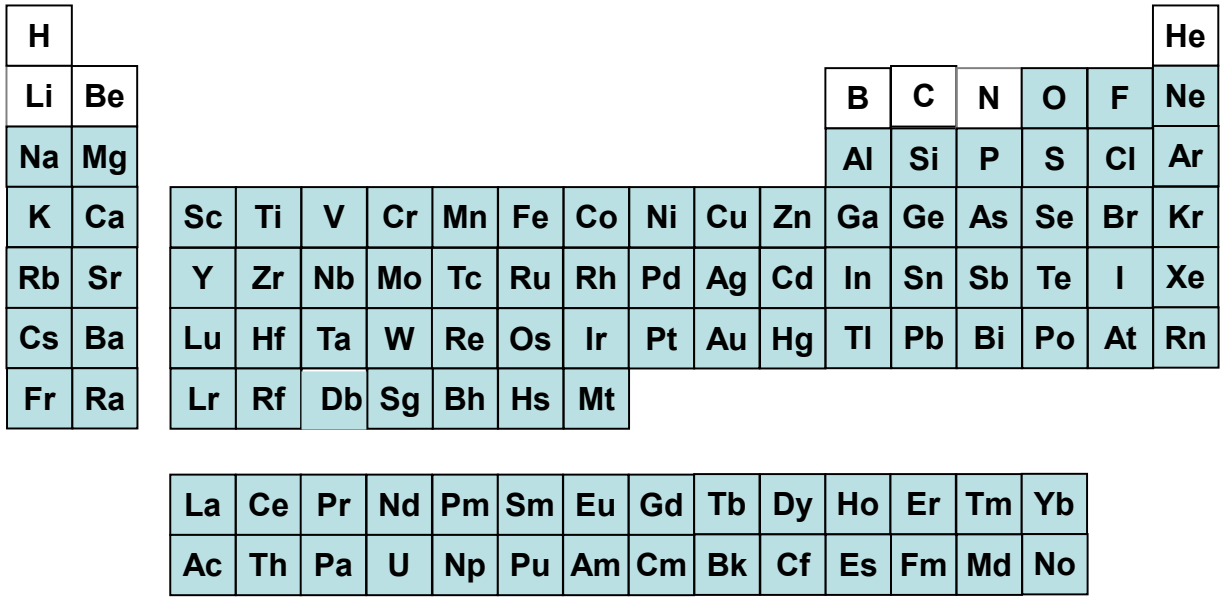
Isotopes and absorption edges – routes to chemical specificity



Elements with absorption edges suitable for EXAFS investigation of local structure in solutions

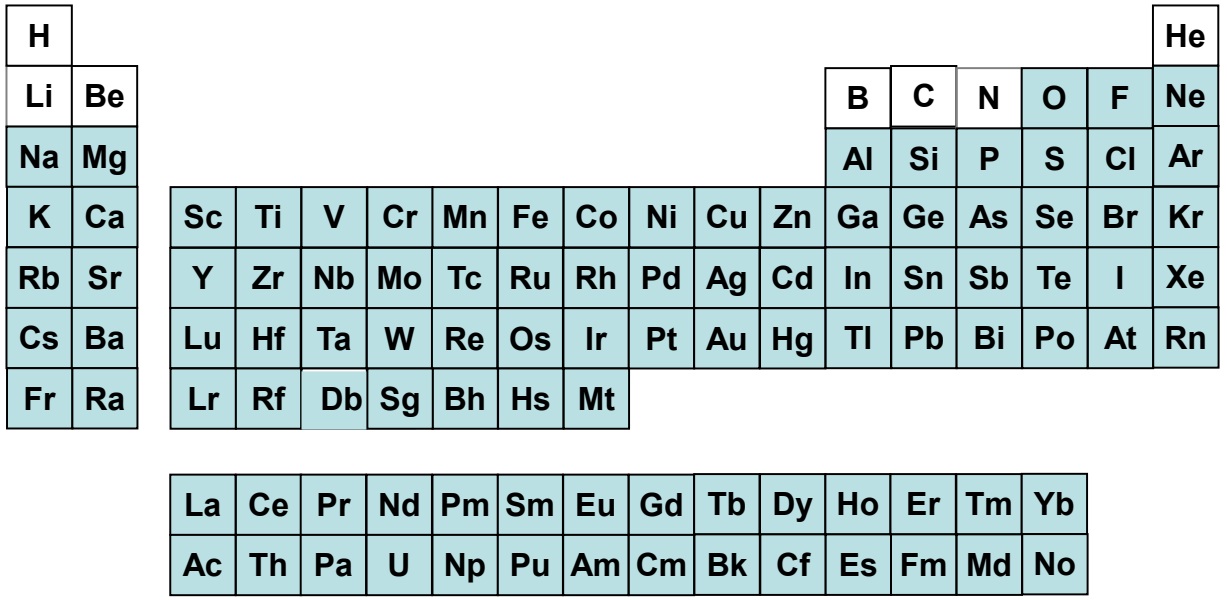
Isotopes and absorption edges – routes to chemical specificity



Elements with absorption edges suitable for EXAFS investigation of local structure in solutions

Concentration limits:

Isotopes and absorption edges – routes to chemical specificity



Elements with absorption edges suitable for EXAFS investigation of local structure in solutions

Concentration limits: Diffraction 1 to 10 atom %

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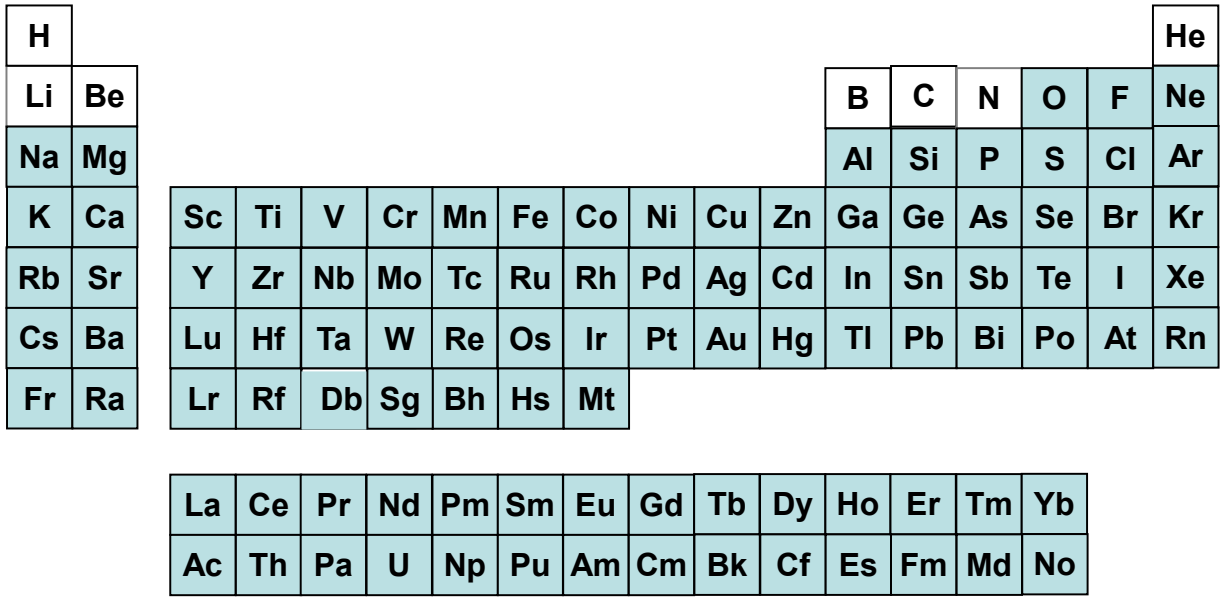
Isotopes and absorption edges – routes to chemical specificity



Elements with absorption edges suitable for EXAFS investigation of local structure in solutions

Concentration limits: Spectroscopy ~ 0.01 atom %

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Benefits of the neutron (or X-ray) scattering plus EXAFS, EPSR analysis approach

(1) Produces a model that is consistent with both bulk and local structural information.
(2) Brings dilute component sensitivity of the spectroscopic probe to bulk structural models.
(3) Circumvents the traditional limitations of direct EXAFS analysis of disordered materials data:
(i) No need for peak shape approximations
(ii) No need for Debye-Waller factor models
(iii) Reduces the number of free parameters in the model to 1
(iv) Provides an unambiguous means to incorporate higher order correlation functions into a disordered materials analysis – sensitivity to the local atomic environmental geometry

Benefits of the neutron (or X-ray) scattering plus EXAFS, EPSR analysis approach

(4) Allows pair potential models to be investigated and refined
(5) Is cheaper, more sensitive and more versatile than neutron scattering with exotic isotopic substitution methods for the investigation of ionic species
(6) Experimentally much simpler and more sensitive than Anomalous X-ray Scattering techniques

If the scattering and spectroscopy data exist, the method can be applied.

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To conclude and for completeness... the EPSR predicted EXAFS of silica glass

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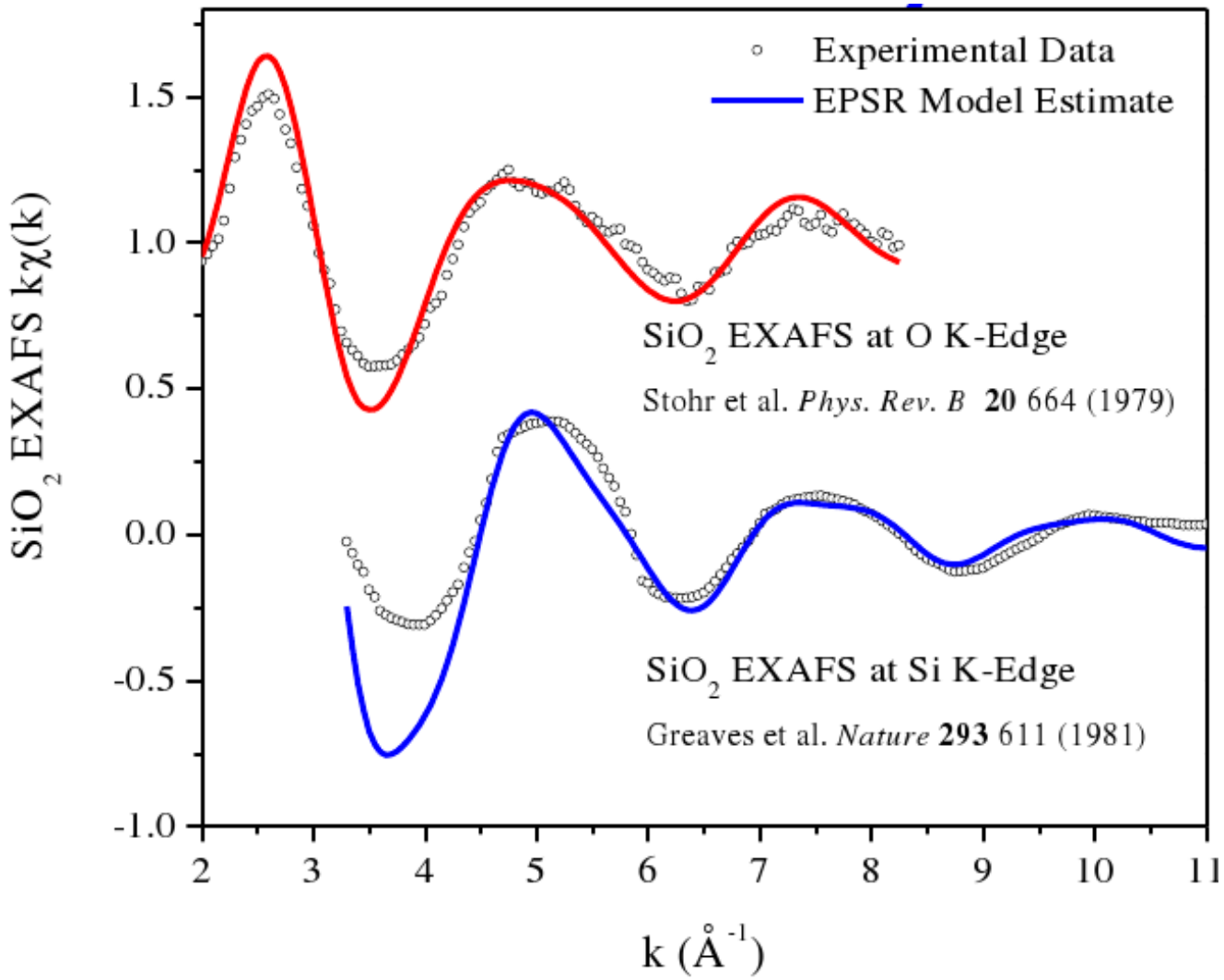
Si and O K-edge EXAFS calculated from EPSR refinement of SiO_2 glass



O-O and O-Si correlations

Si-Si and Si-O correlations

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Sofía Díaz Moreno — **Diamond Light Source, UK**

EPSR-EXAFS references

D.T.Bowron and S.Díaz-Moreno *J. Phys. Chem. B*, **111** 11393 (2007)

D.T.Bowron, *Pure Appl. Chem.* **80** 1211 (2008)

D.T.Bowron, *Mat. Sci. Eng. B*, **149** 166 (2008)