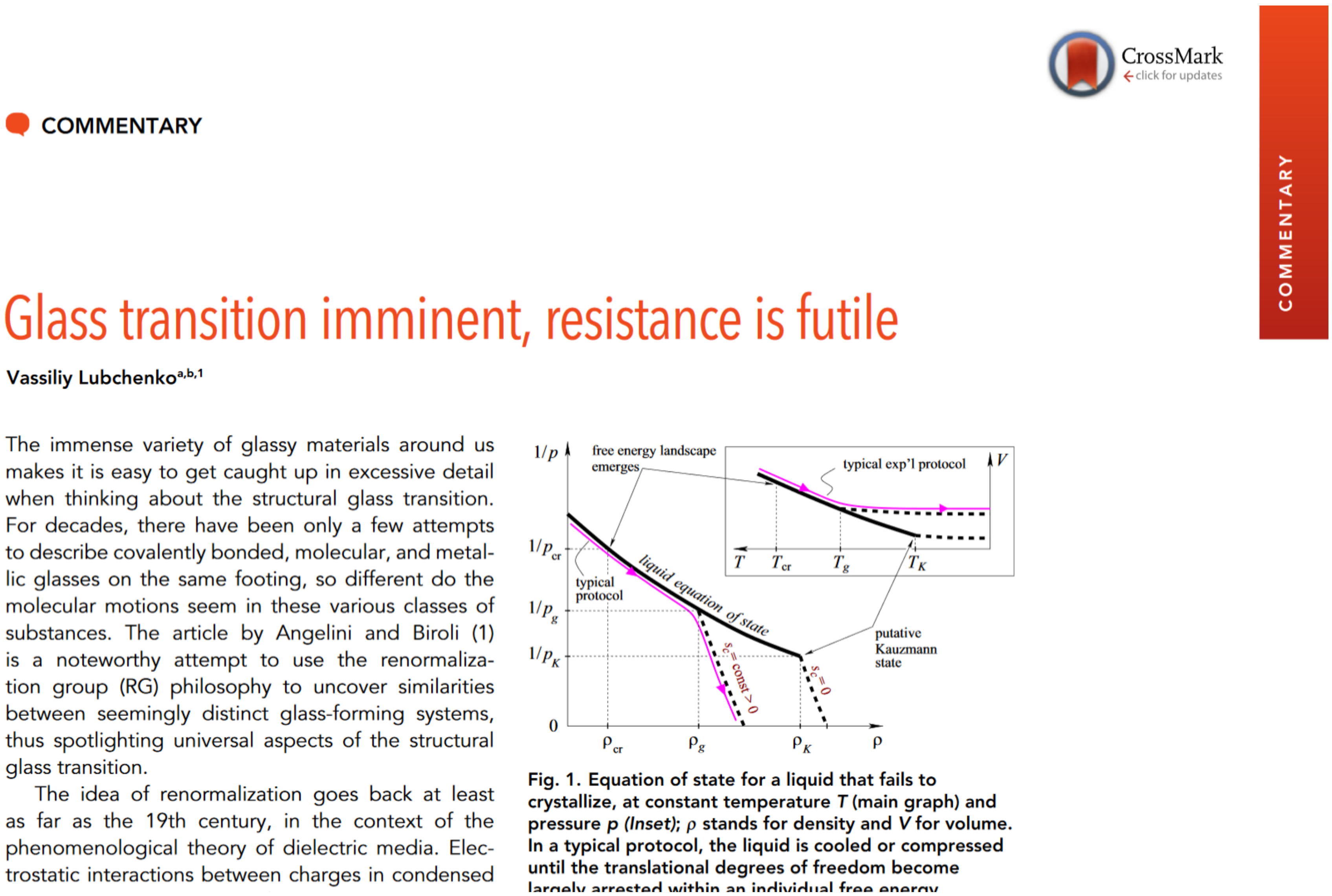

COMMENTARY

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click for updates

COMMENTARY

Glass transition imminent, resistance is futile

Vassiliy Lubchenko[a,b,1]

The immense variety of glassy materials around us makes it is easy to get caught up in excessive detail when thinking about the structural glass transition. For decades, there have been only a few attempts to describe covalently bonded, molecular, and metallic glasses on the same footing, so different do the molecular motions seem in these various classes of substances. The article by Angelini and Biroli (1) is a noteworthy attempt to use the renormalization group (RG) philosophy to uncover similarities between seemingly distinct glass-forming systems, thus spotlighting universal aspects of the structural glass transition.

The idea of renormalization goes back at least as far as the 19th century, in the context of the phenomenological theory of dielectric media. Electrostatic interactions between charges in condensed

Fig. 1. Equation of state for a liquid that fails to crystallize, at constant temperature T (main graph) and pressure p *(Inset)*; ρ stands for density and V for volume. In a typical protocol, the liquid is cooled or compressed until the translational degrees of freedom become largely arrested within an individual free energy

PNAS, 20 mars 2017

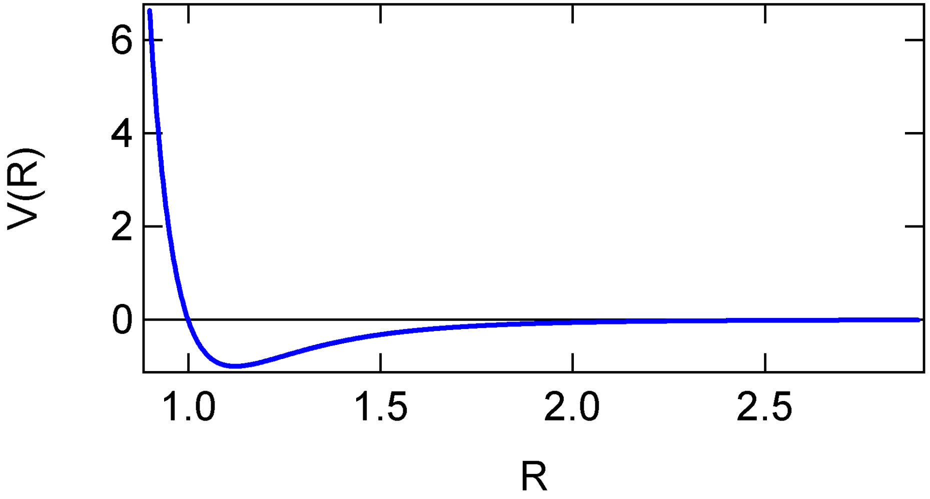
Bertrand has generated sets of (x,y,z) positions for various times at various given thermodynamic conditions (N,V,T,P). Matthieu attempts now to use the trajectories !

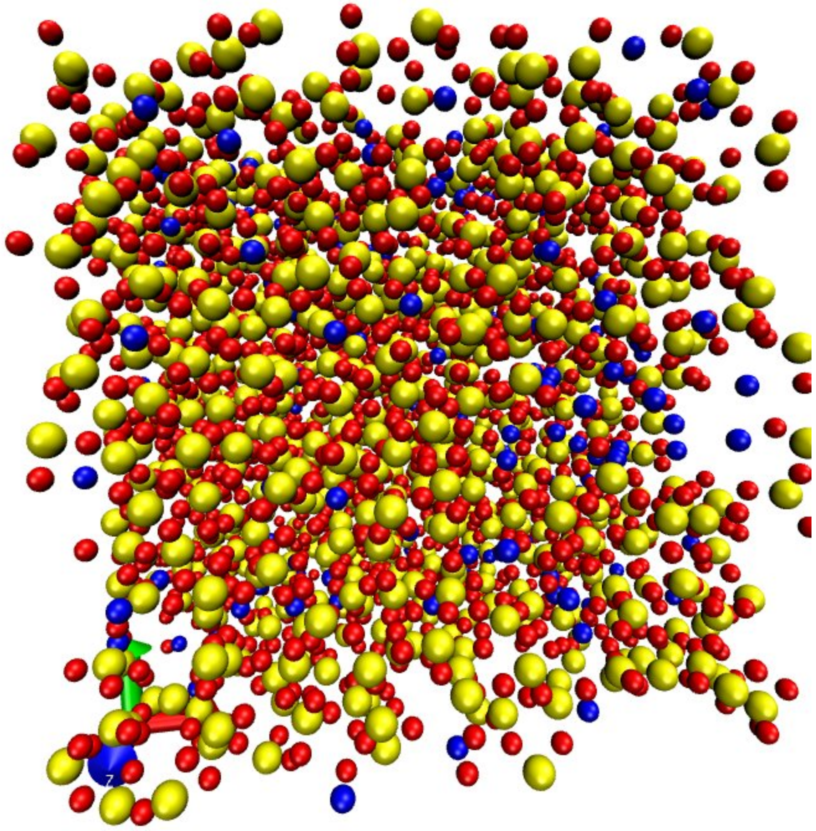
Numerical simulations and Rigidity of glasses – I

Matthieu Micoulaut (UPMC)

- What can we obtain from MD trajectories ?
    - Structure
    - Dynamics

matthieu.micoulaut@upmc.fr



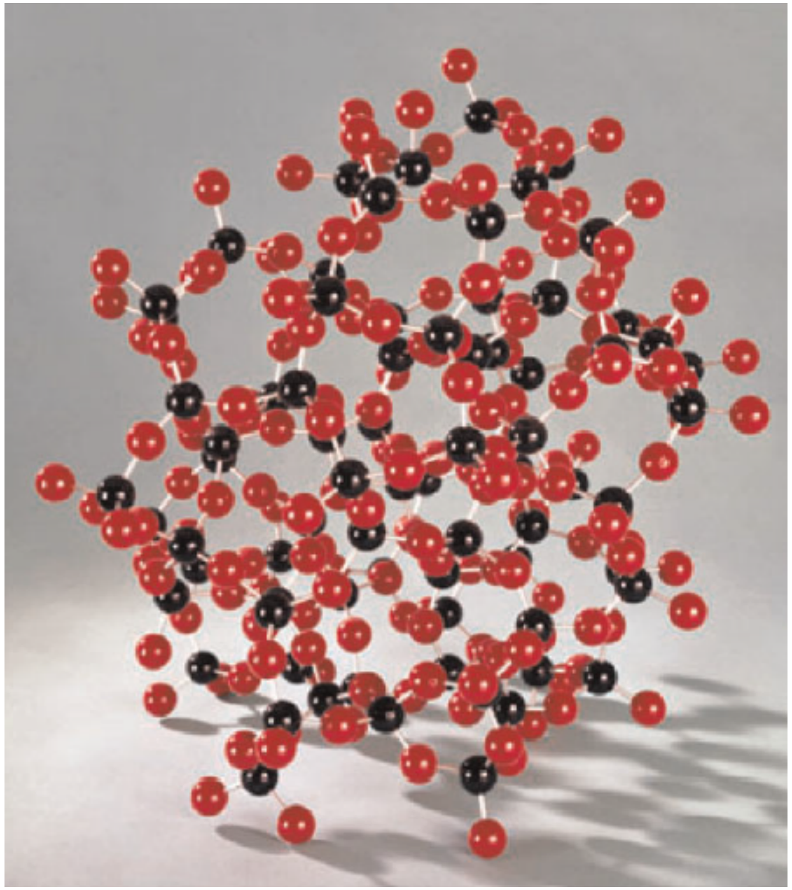


$x_i(t), y_i(t), z_i(t)$ →

Structure
Thermodynamique
Dynamique
Vibration

Historically…

Compution of the radial distribution function of vitreous SiO_2 from a ball and stick model



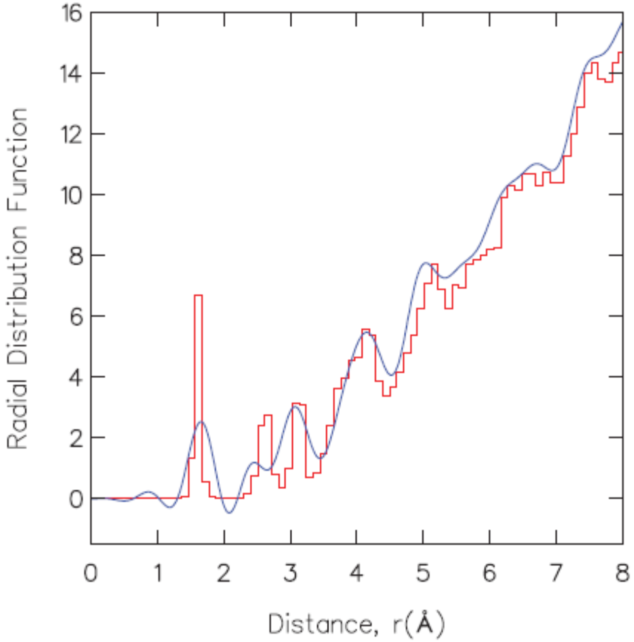
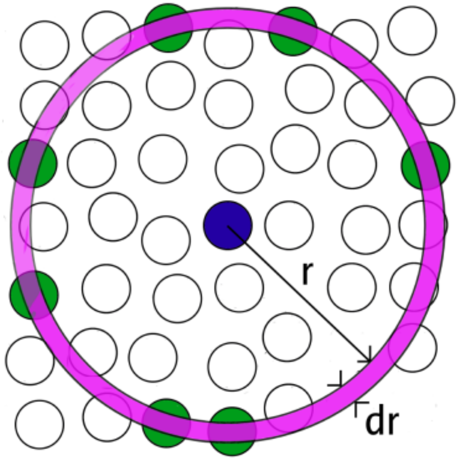


Figure 4 (online colour at: www.pss-b.com) A comparison of the relaxed [9] Bell and Dean [4] model (1980) for vitreous silica (red histogram) with X-ray data (blue curve). The histogram does not include thermal broadening, nor the experimental broadening in real space, whilst the X-ray data of Mozzi and Warren [6] have been Fourier transformed to simulate the earlier (1936) Radial Distribution Function of Warren et al. [10].

Bell and Dean, 1972

A) PAIR CORRELATIONS



- ☐ Radial distribution function :

$$g(\boldsymbol{r}) = \frac{1}{N\rho}\sum_{i=1}^{N}\sum_{k\neq i}^{N}\langle\delta(\boldsymbol{r}+\boldsymbol{r}_k-\boldsymbol{r}_i)\rangle$$

- ☐ Pair correlation function:

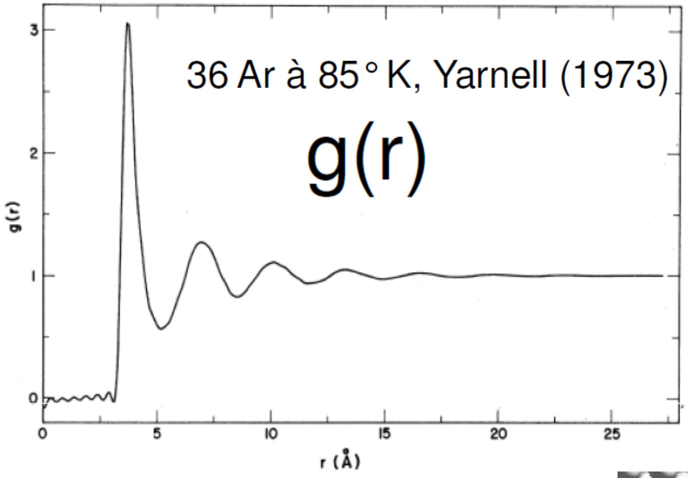
$$g(r) = \frac{1}{4\pi r^2}\frac{1}{N\rho}\sum_{i=1}^{N}\sum_{k\neq i}^{N}\langle\delta(\boldsymbol{r}-|\boldsymbol{r}_k-\boldsymbol{r}_i|)\rangle$$

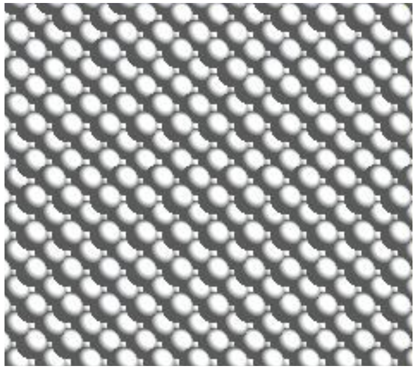
Alternative definitions :

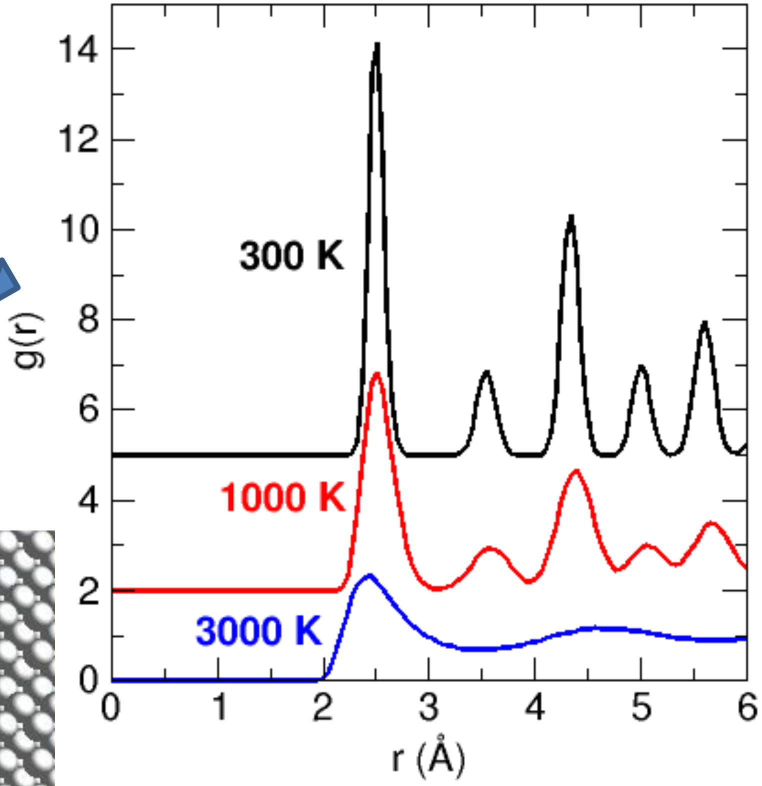
- ☐ Total distribution function: $T(r) = 4\pi\varrho r g(r)$
- ☐ Differential distribution function $D(r) = 4\pi\varrho r[g(r)-1]$

Pair distribution function : examples

Visual inspection allows to distinguish between a crystalline and an amorphous structure







BCC Ni lattice with EAM potential

Effect of thermodynamic variables : temperature

Amorphous Se

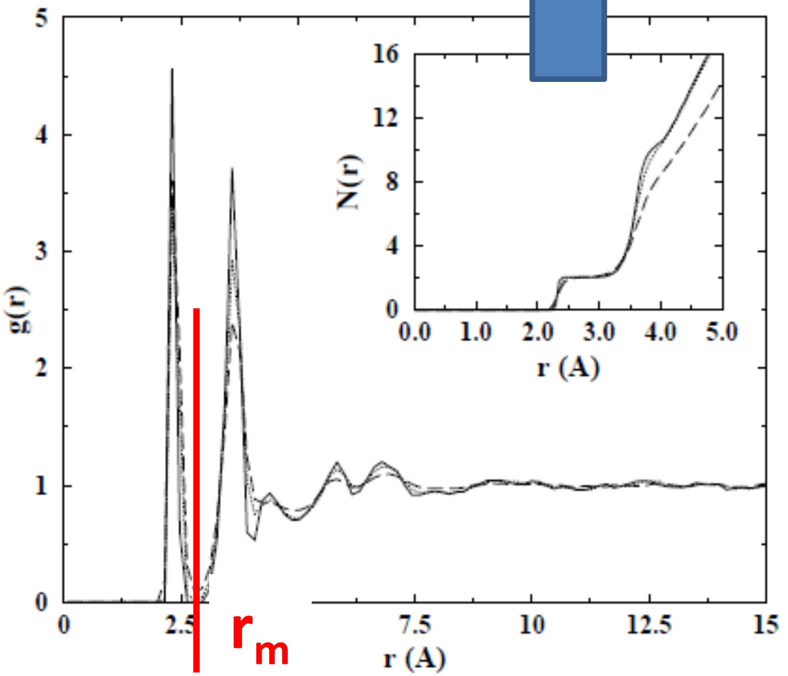


FIG. 3. Pair correlation function of Se at three different temperatures: 6 K (solid line), 290 K (dotted line), 550 K (long dashed line). The inset shows the mean coordination numbers for the same temperatures.

Caprion, Schober, PRB 2000

The integral of g(r) allows to determine the number of neighbors around a central atom.
Remember

$$\int_{r=0}^{\infty} \rho g(r).4\pi r^2 dr = N-1$$

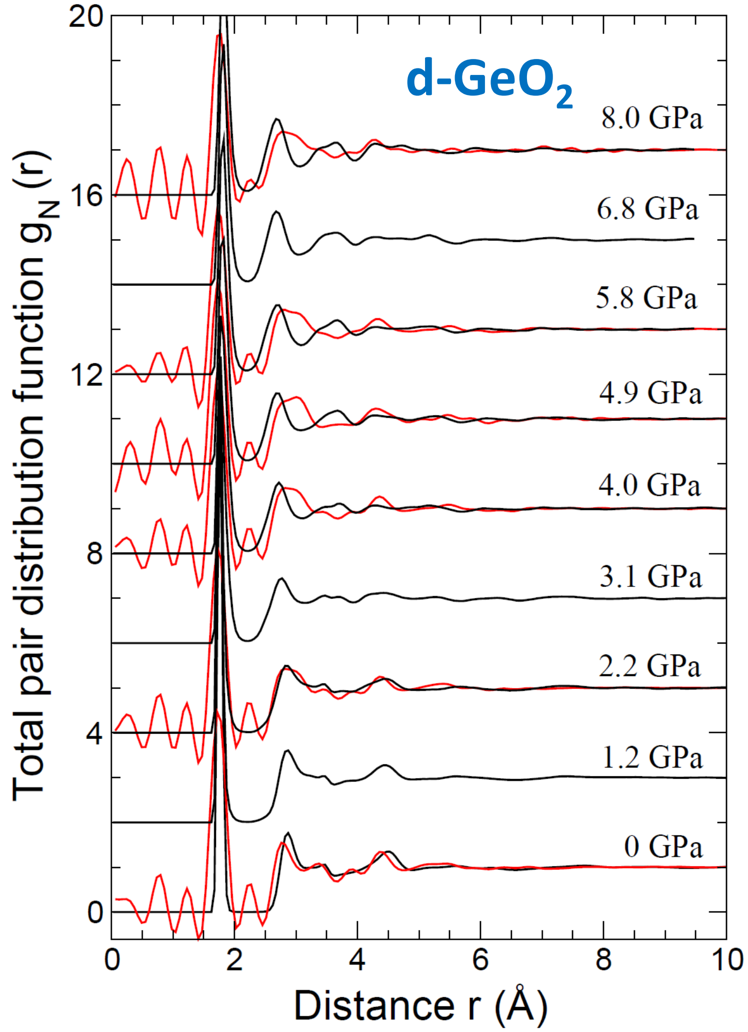
The integral to the first minimum gives the coordination number.

$$\boxed{CN = \int_0^{r_m} \varrho g(r) 4\pi r^2 dr}$$

Running coordination number N(r)

$$N(r) = \int_0^{r} \varrho g(r') 4\pi r'^2 dr'$$

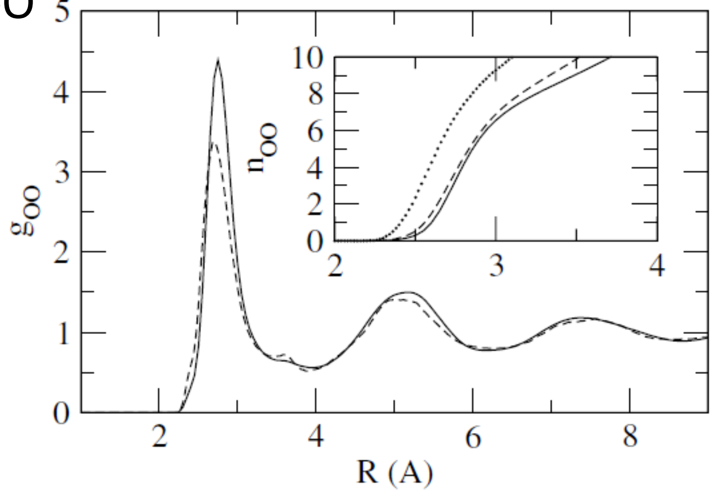
Effect of thermodynamic variables : pressure



Expt. (neutron) Salmon, JPCM 2011

MD: 256 GeO$_2$ using Oeffner-Elliot FF

- ☐ Direct comparison with experiments possible but can sometimes fail
- ☐ Simple force fields can not account for pressure-induced changes (metallization)
- ☐ Additional structural insight is provided by partial correlation functions : Ge-Ge, Ge-O, O-O

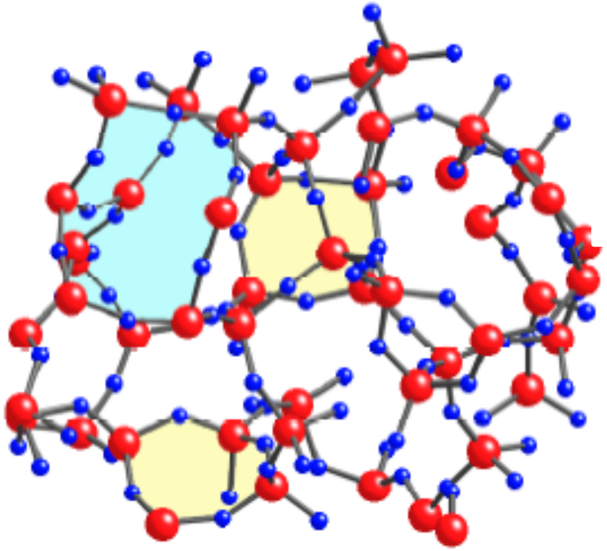


Micoulaut, JPCM 2004

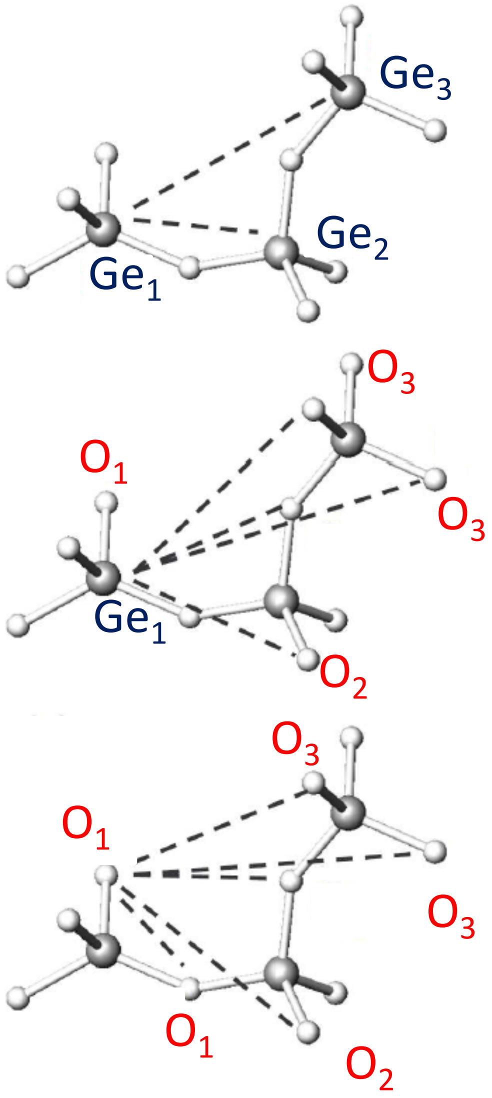
Effect of composition: extending to multicomponent systems

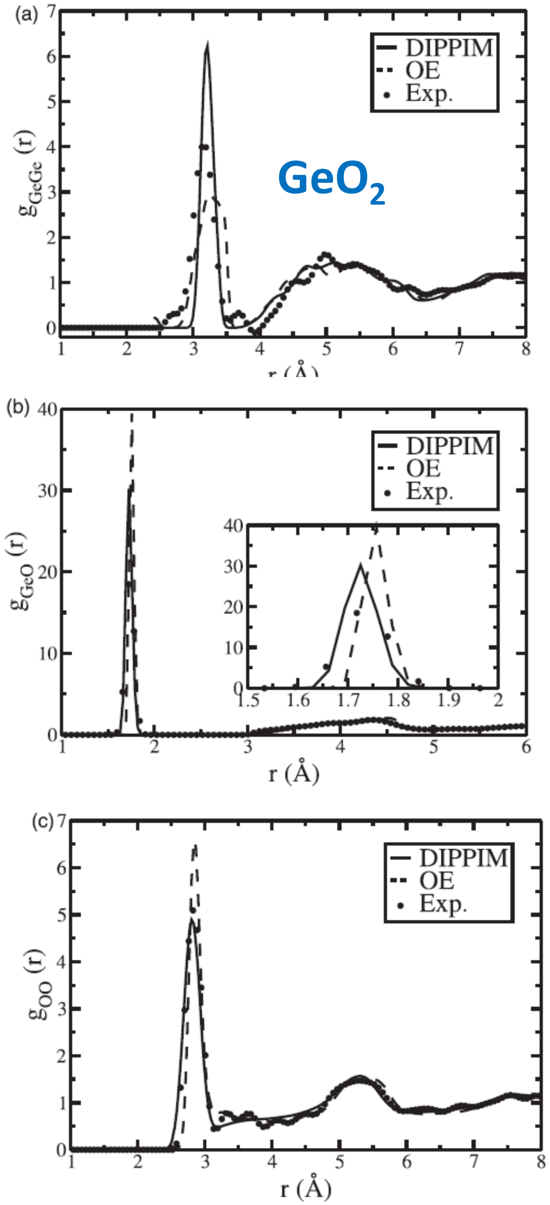
This is case for most glasses and materials

SiO_2, $GeSe_2$, SiO_2-Na_2O,…



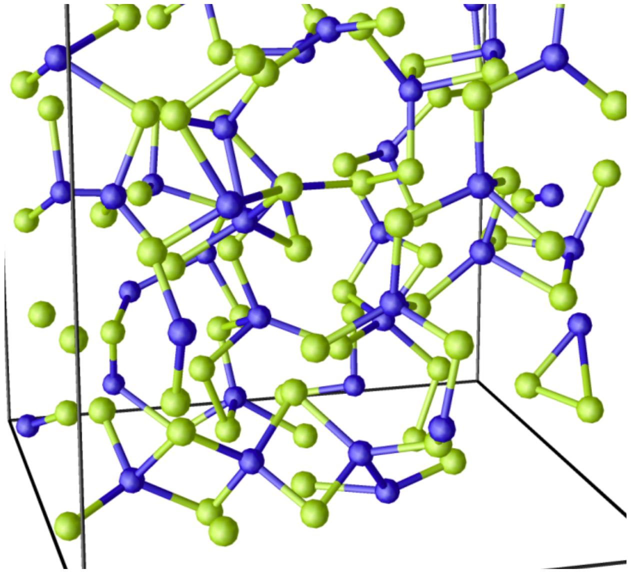
D. Marrocchelli et al., 2010

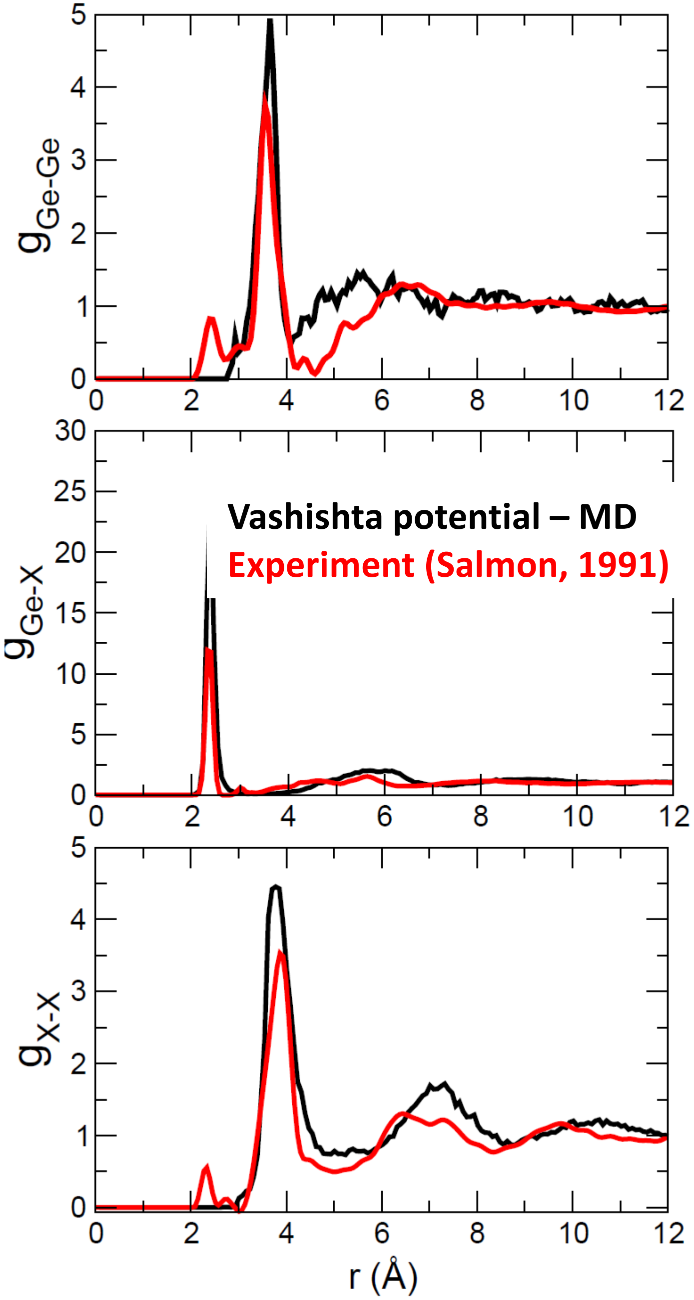




Pair distribution function in multicomponent systems…failures

GeSe$_2$

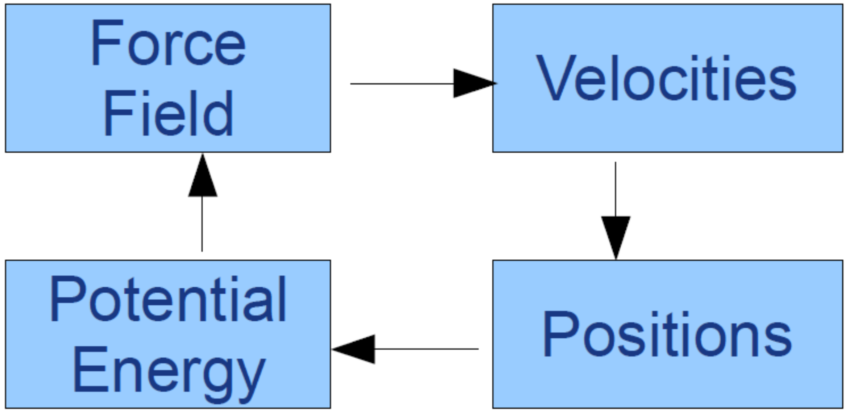




- **Need to use First Principles Molecular Dynamics**
  - Classical force field fail to describe the structure
  - Charge transfer (covalent bonding)
  - Homopolar defects

First Principles Molecular Dynamics simulations of chalcogenides

Classical MD



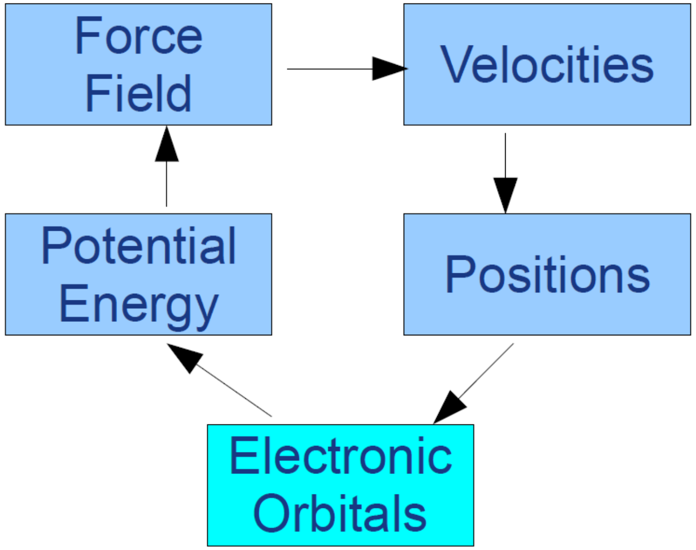
Force Field

Velocities

Positions

Potential Energy

Ab initio MD



Force Field

Velocities

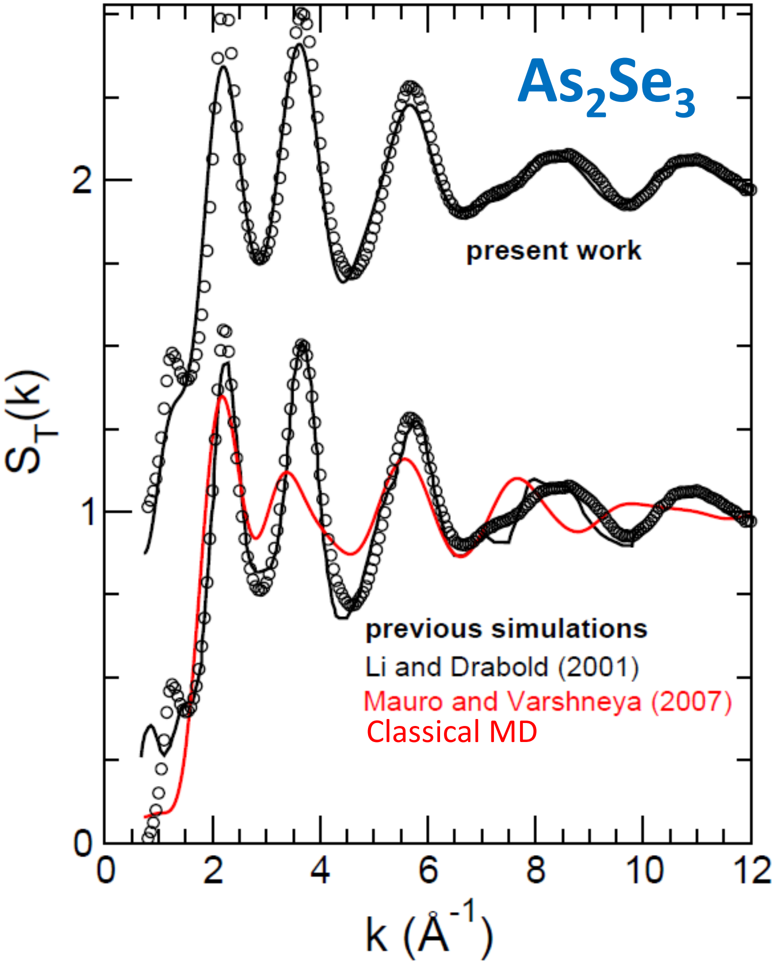
Positions

Electronic Orbitals

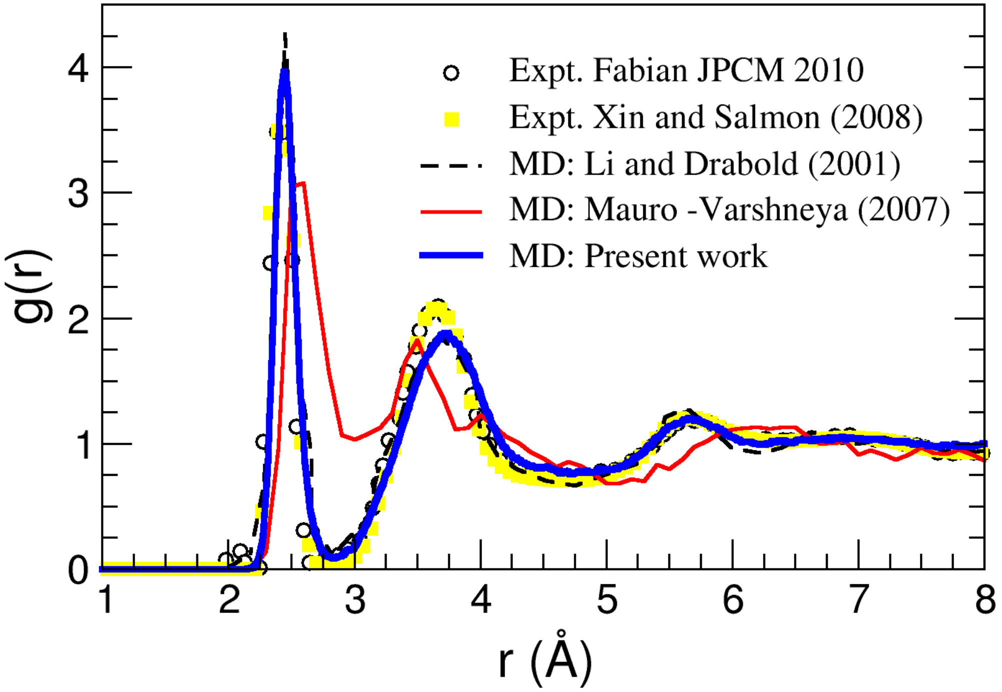
Potential Energy

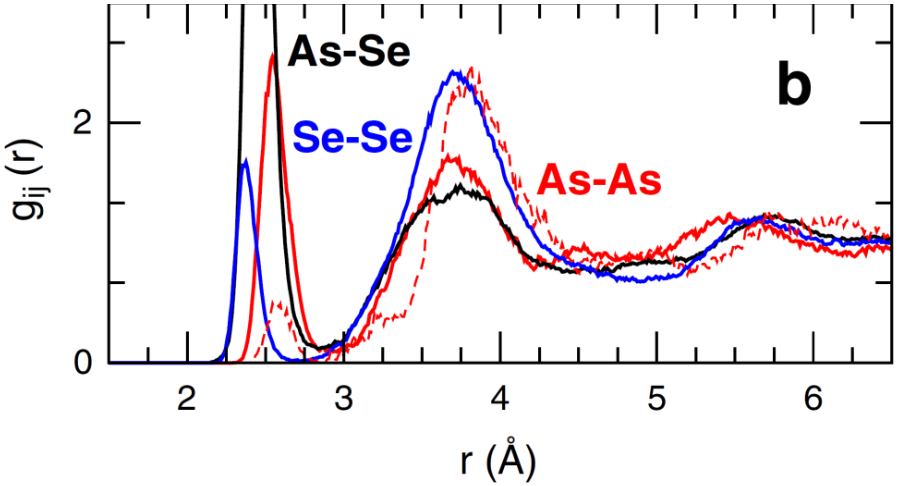
Solve the Schroedinger equation for a system of N atoms
Simplified with the DFT scheme (one electron density)

☐ No force field necessary. Heavy computational cost
☐ Small systems (100s of atoms, 10^6 in Classical MD)
☐ Small simulation time (100ps, 100 ns for classical MD)
☐ Most approximation encoded in the exchange-correlation functional



Bauchy et al. JNCS 2013





Presence of homopolar defects !!

B) STATIC STRUCTURE FACTOR

For a simple liquid, the static structure factor is given by : $S(\mathbf{k}) = \frac{1}{N}\langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle$

where ρ_k is the Fourier transform of the microscopic density $\rho(\mathbf{r})$.
In molecular simulations, a convenient way of calculating is:

$$\boxed{S(\mathbf{k}) = \frac{1}{N}\left\langle \sum_{i=1}^{N} \sum_{j=1}^{N} \exp(-i\mathbf{k}\mathbf{r}_i) \exp(i\mathbf{k}\mathbf{r}_j) \right\rangle .}$$

$$S(\mathbf{k}) = 1 + \frac{\rho^2}{N} \int \int \exp(-i\mathbf{k}(\mathbf{r} - \mathbf{r}'))g(\mathbf{r}, \mathbf{r}')d\mathbf{r}d\mathbf{r}'$$

Also, g(**r**,**r’**) depends only on |**r-r’**|, i.e.: $S(\mathbf{k}) = 1 + \rho \int \exp(-i\mathbf{k}\mathbf{r})g(r)d\mathbf{r}.$

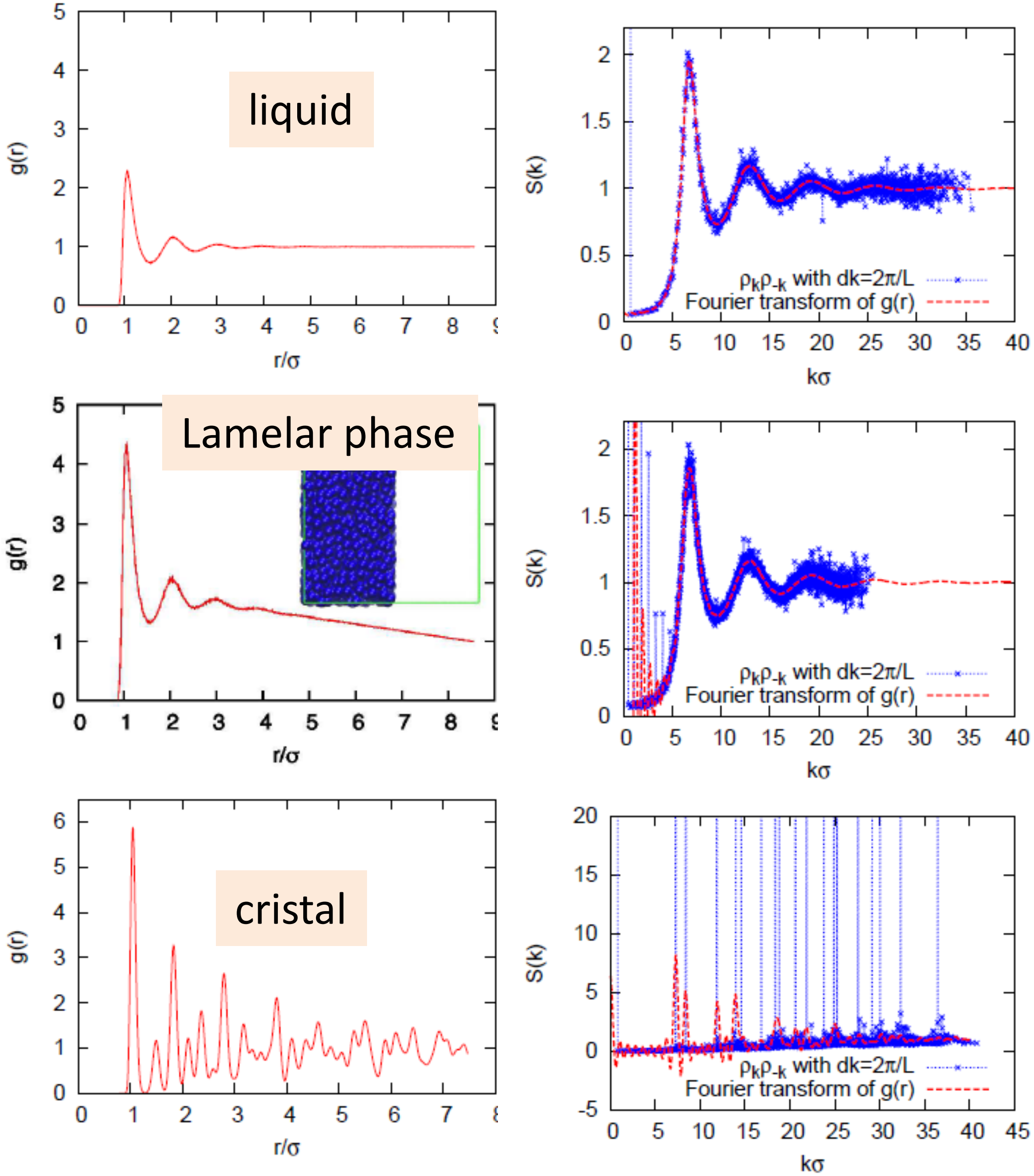
Or (isotropic fluid, everything depends only on k=|**k**|):

$$\boxed{S(k) = 1 + 4\pi\rho \int_0^{\infty} r^2 g(r) \frac{\sin(kr)}{kr} dr.}$$

An alternative calculation of the structure factor S(k) is achieved via a Fourier transform of the pair distribution function g(r).

In a cubic box of finite size L with PBC with periodic boundary conditions (PBCs)

- wavevector increment is $\delta k = 2\pi/L$
- PBCs impose a constraint L on the maximum possible period.
- Any period larger than L (any wavevector smaller than k) is unphysical.
- For glasses, uniformity hypothesis
- Both methods agree for **liquids and glasses**
- FT breaks down for the low k limit (long wavenumber **lamellar phase**)
- For **crystals**, the FT of g(r) only capture some peak locations of S(k).
- Peak locations that correspond only partially to those determined from crystallography (blue vertical lines)

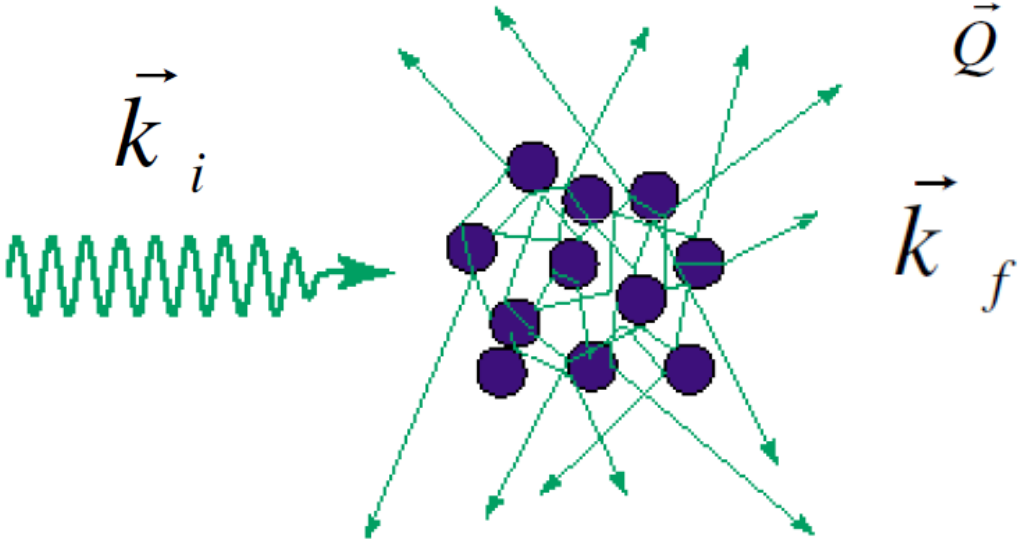


Lennardjonesium

Zhang, arXiv:1606.03610v2 (2016)

Direct comparison with experiments : neutron or X-ray diffraction

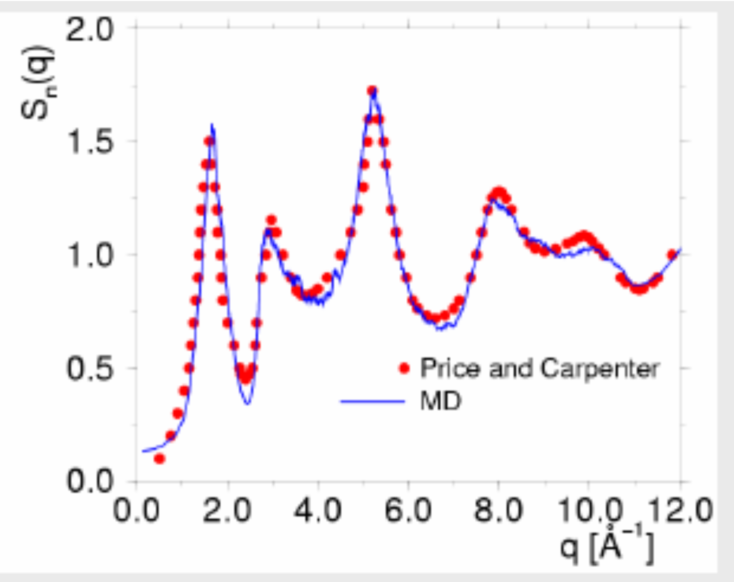
$$\vec{Q} = \vec{k}_f - \vec{k}_i$$



Intensity scattered in the direction k_f

$$I(\vec{Q}) \propto S(\vec{Q}) = \frac{1}{N}\left\langle \left| \sum_{i=1}^{N} \exp(i\vec{Q}.\vec{r}_i) \right|^2 \right\rangle = \frac{1}{N}\left\langle \sum_{i=1}^{N}\sum_{j=1}^{N} \exp(i\vec{Q}.(\vec{r}_i - \vec{r}_j)) \right\rangle$$

Equal to the computed structur efactor.



Kob et al. 1999

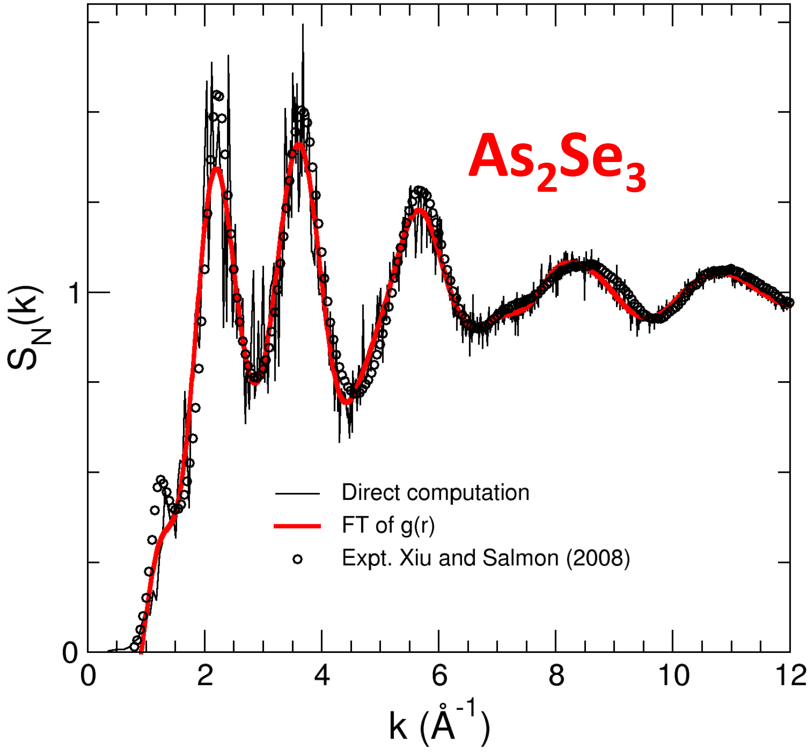
Calculating a structure factor S(k) from a MD simulation : 2 options

1. Calculate the pair correlation function g(r) from the MD trajectory, then use :

$$S(k) = 1 + 4\pi\rho \int_0^{\infty} r^2 g(r) \frac{\sin(kr)}{kr} dr.$$

2. Calculate directly S(k) from the trajectory using:

$$S(\mathbf{k}) = \frac{1}{N} \left\langle \sum_{i=1}^{N} \sum_{j=1}^{N} \exp(-i\mathbf{k}\mathbf{r}_i) \exp(i\mathbf{k}\mathbf{r}_j) \right\rangle .$$



Differences between both methods can arise, and one is limited to r<L/2, i.e. **$k<\pi/L$**

Effects of the components of the wavevector

Structure factor in multicomponent systems

SiO_2, $GeSe_2$, SiO_2-Na_2O,…

Consider a system with n components having N_1, N_2, …N_n particles.
We can write Faber-Ziman partial structure factors:

$$S_{\alpha\beta}(\boldsymbol{k}) = \frac{(1+\delta_{\alpha\beta})}{2N}\sum_{i=1}^{N_\alpha}\sum_{k\neq i}^{N_\beta}\langle \exp[-\boldsymbol{k}.(\boldsymbol{r}_i-\boldsymbol{r}_k)]\rangle$$

out of which can be computed a total structure factor:

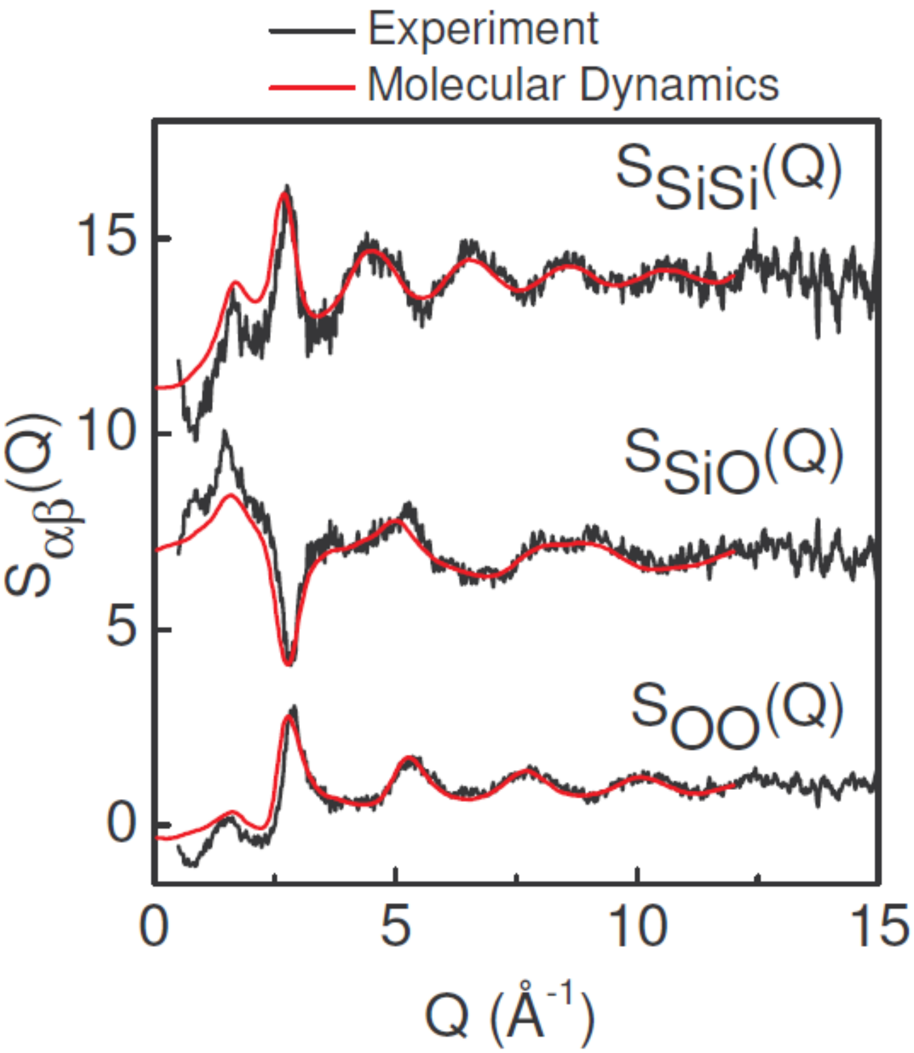
- **Neutron weighted**: $S_N(k) = \dfrac{\sum_{i,j} c_i c_j b_i b_j S_{ij}(k)}{\sum_{i,j} c_i c_j b_i b_j}$

with b_i the neutron scattering cross section , c_i the concentration of the species
b_i= (tabulated, depends on the isotope)

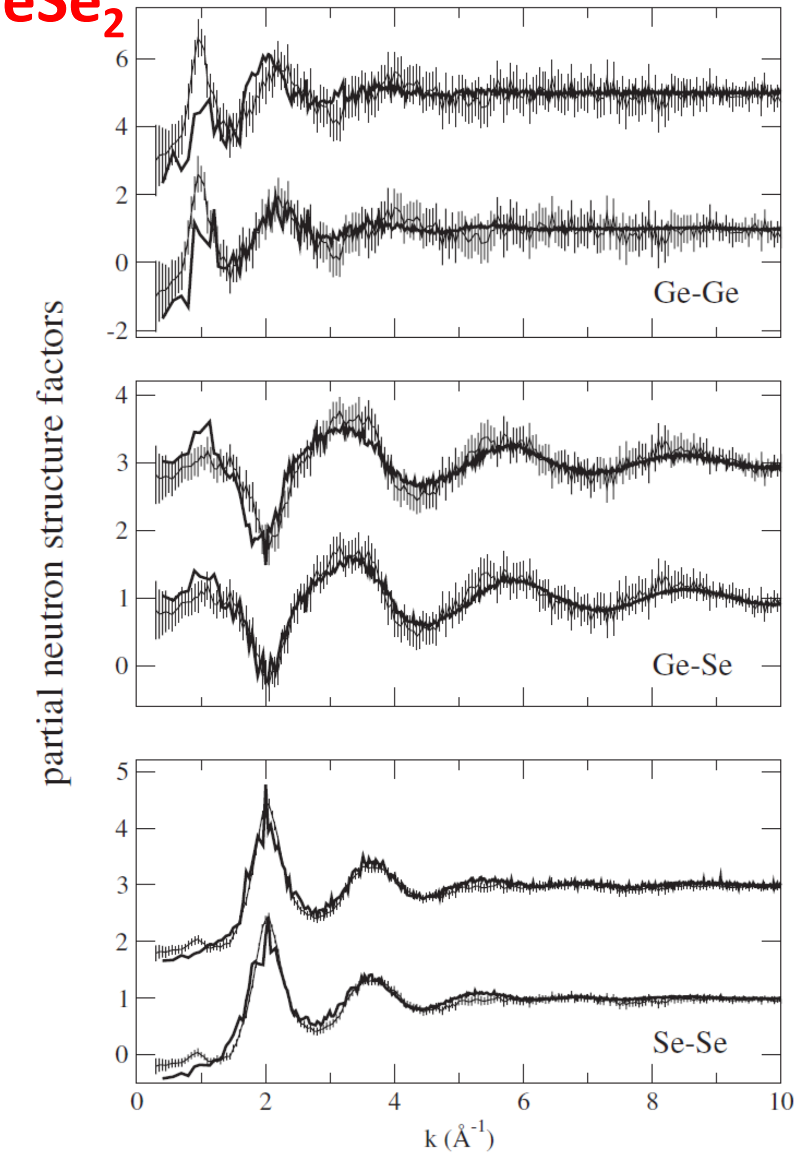
- **X-ray weighted:** $S_N(k) = \dfrac{\sum_{i,j} c_i c_j f_i(k) f_j(k) S_{ij}(k)}{\sum_{i,j} c_i c_j f_i(k) f_j(k)}$

With $f_i(k)$ the X-ray form factor (elastic or inelastic XRD)

v-SiO_2 Phys. Rev. B. 78 (2008) 144204 .



l-$GeSe_2$



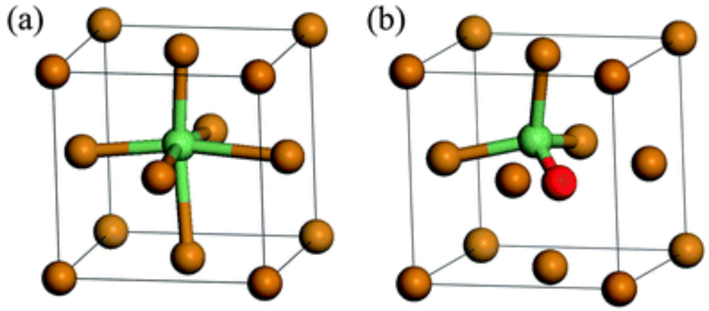
Micoulaut et al., PRB 2009

Detailed structural analysis from MD

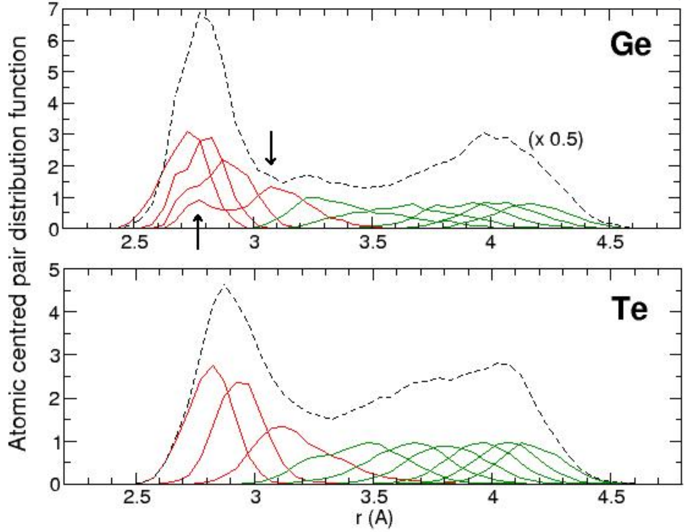
☐ Neighbor distribution

Remember $$CN = \int_0^{r_m} \varrho g(r) 4\pi r^2 dr$$

First minimum of g(r) can be used to define the coordination number.
But this is an average.



Amorphous $Ge_1Sb_2Te_4$



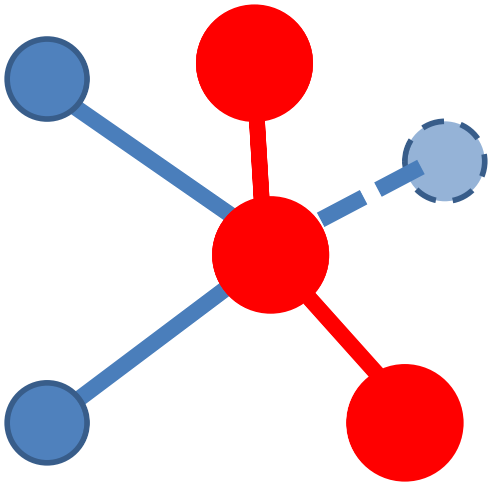
- Details are provided from the statistical analysis of each atom.
- Allows to characterize the nature of the neighborhood
- Can be extended to partial CN

Raty et al. Solid State Sciences 2010

$$CN_{ij} = \int_0^{r_m} \varrho g_{ij}(r) 4\pi r^2 dr$$

Examples-2: Statistics of neighbors with homopolar bonds

$Ga_{11}Ge_{11}Te_{78}$



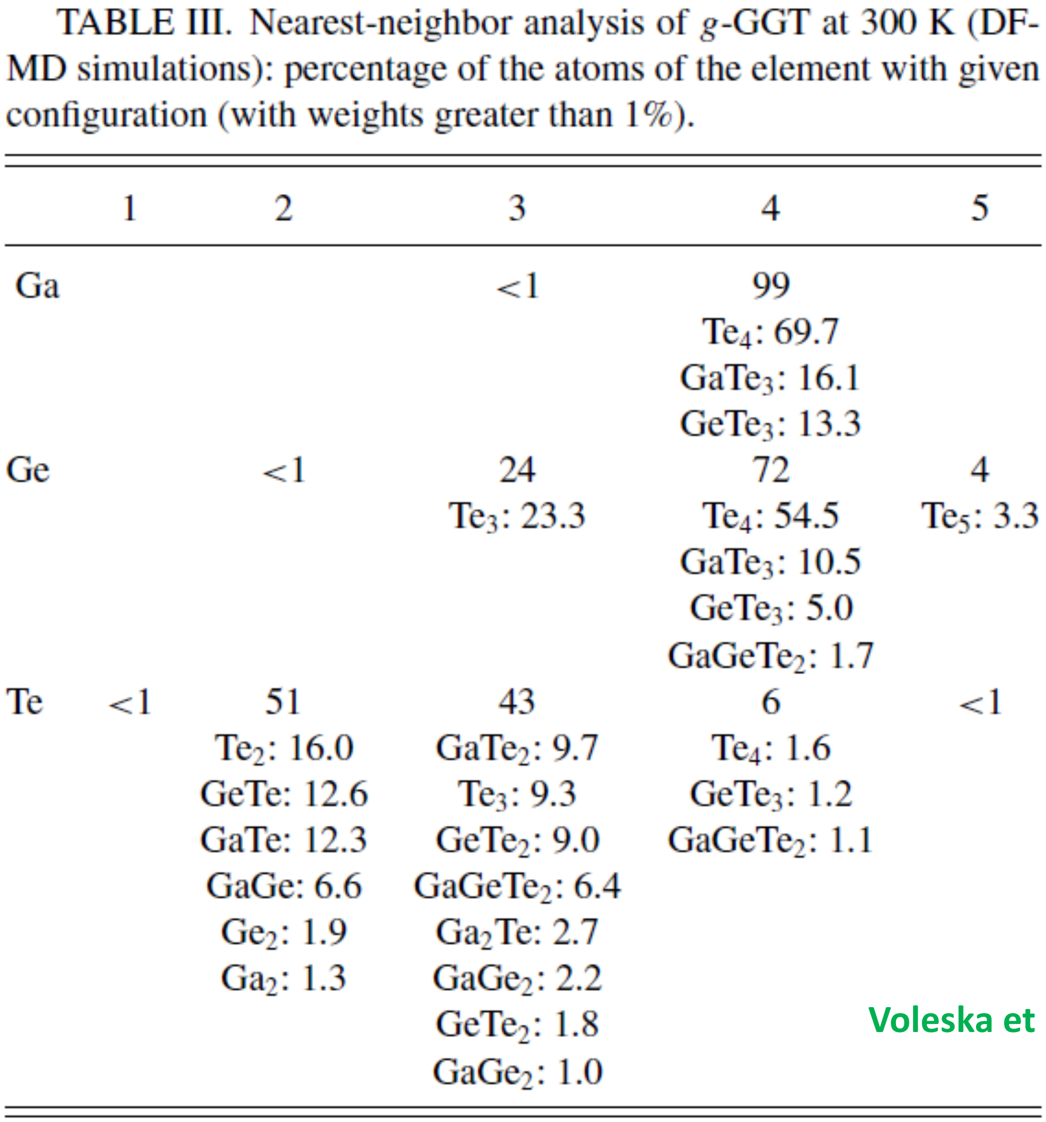


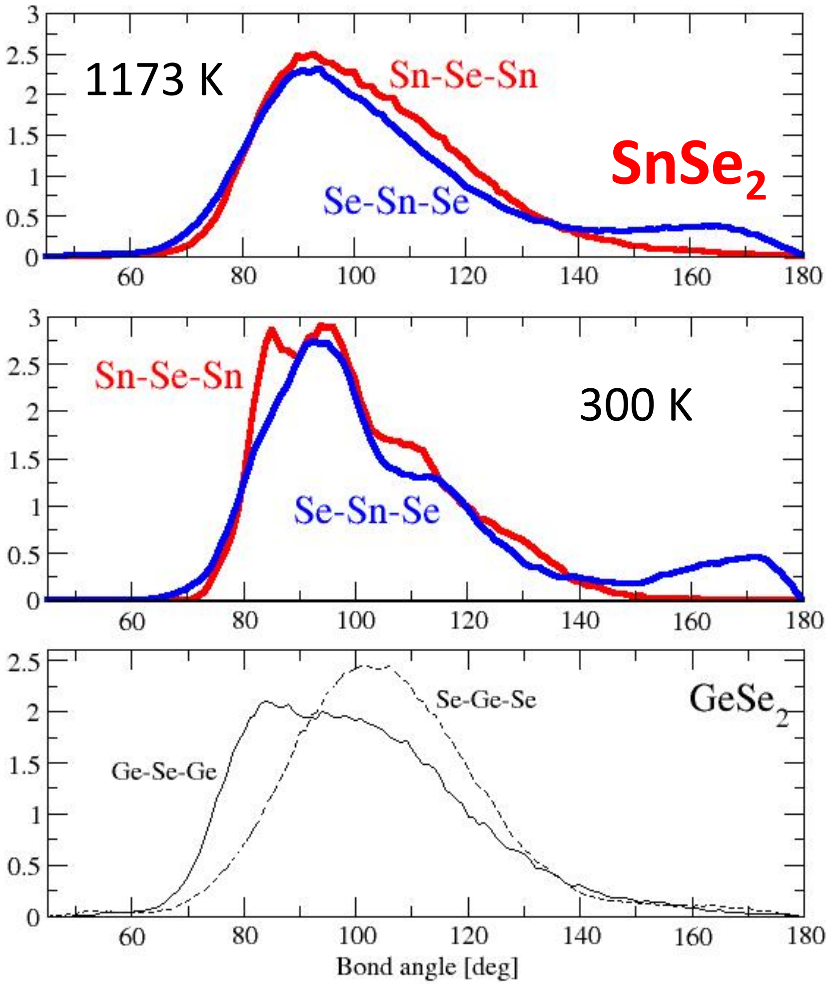
TABLE III. Nearest-neighbor analysis of *g*-GGT at 300 K (DF-MD simulations): percentage of the atoms of the element with given configuration (with weights greater than 1%).

	1	2	3	4	5
Ga			<1	99 Te_4: 69.7 $GaTe_3$: 16.1 $GeTe_3$: 13.3	
Ge		<1	24 Te_3: 23.3	72 Te_4: 54.5 $GaTe_3$: 10.5 $GeTe_3$: 5.0 $GaGeTe_2$: 1.7	4 Te_5: 3.3
Te	<1	51 Te_2: 16.0 GeTe: 12.6 GaTe: 12.3 GaGe: 6.6 Ge_2: 1.9 Ga_2: 1.3	43 $GaTe_2$: 9.7 Te_3: 9.3 $GeTe_2$: 9.0 $GaGeTe_2$: 6.4 Ga_2Te: 2.7 $GaGe_2$: 2.2 $GeTe_2$: 1.8 $GaGe_2$: 1.0	6 Te_4: 1.6 $GeTe_3$: 1.2 $GaGeTe_2$: 1.1	<1

Voleska et al., PRB 2013

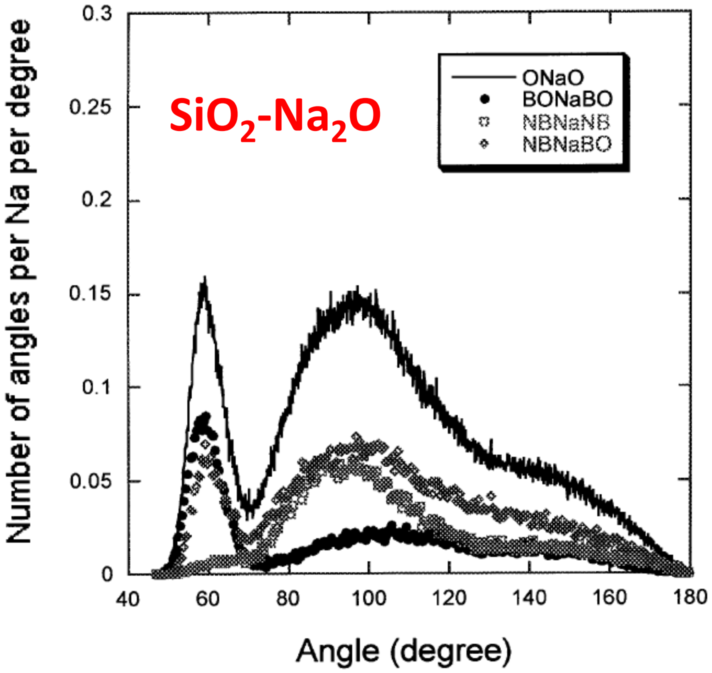
Detailed structural analysis from MD

- ☐ Bond angle distributions



Micoulaut et al. PRB 2008

- ☐ Depending on the system, provides information about the local geometry (tetrahedral, octahedral,…).
- ☐ Directional bonding vs non-directional



Cormack and Du, JNCS 2001

Detailed structural analysis from MD

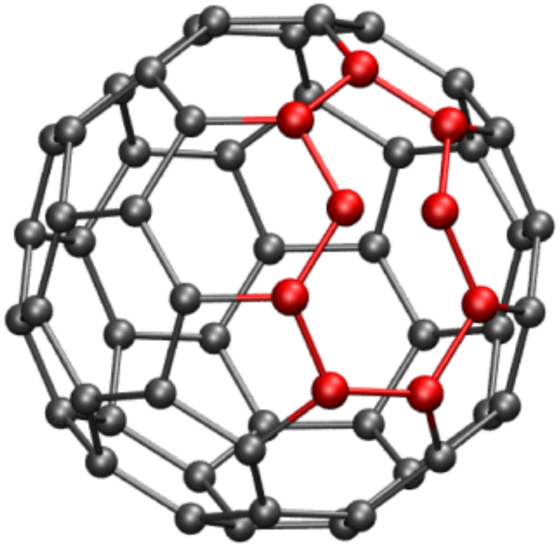
☐ Ring statistics: serve to characterize the intermediate range order

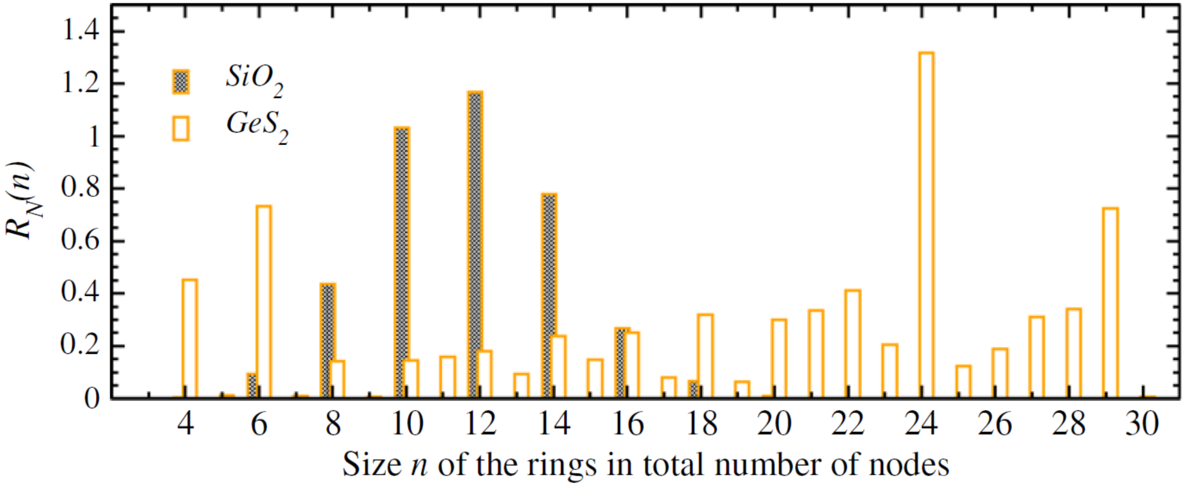
- Simulated positions can serve to define nodes and links.

  When connected sequentially without overlap, one has a path.

  A ring is therefore simply a closed path.

  Each of these rings is characterized by its size and can be classified.





S. Le Roux, P. Jund, Comp. Mater. Sci. 2010

http://rings-code.sourceforge.net/

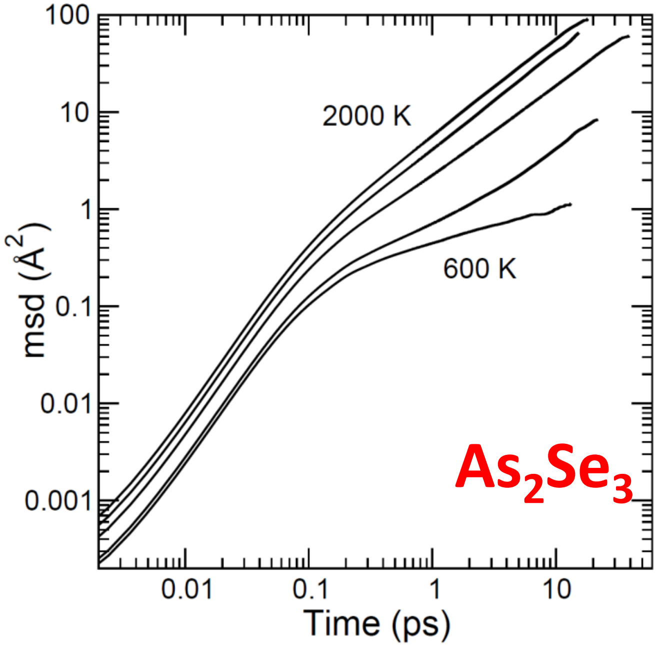
C) MEAN SQUARE DISPLACEMENT AND DIFFUSION

The mean square displacement is defined as

$$\langle r^2(t)\rangle = \frac{1}{N_\alpha}\sum_{i=1}^{N_\alpha}\langle|r_i(t)-r_i(0)|^2\rangle,$$

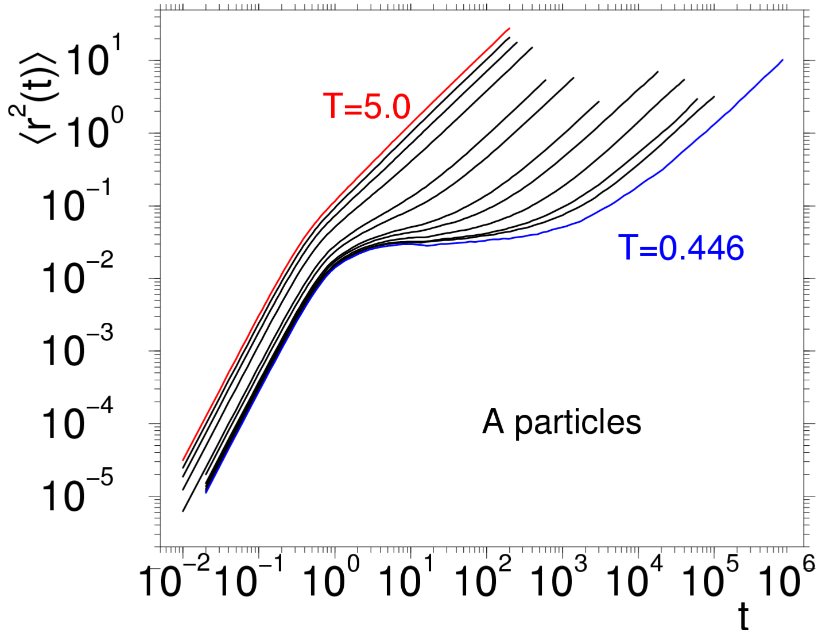
- performed in NVE or NVT.
- do not use periodic boundary conditions

Gives a direct description of the dynamics.



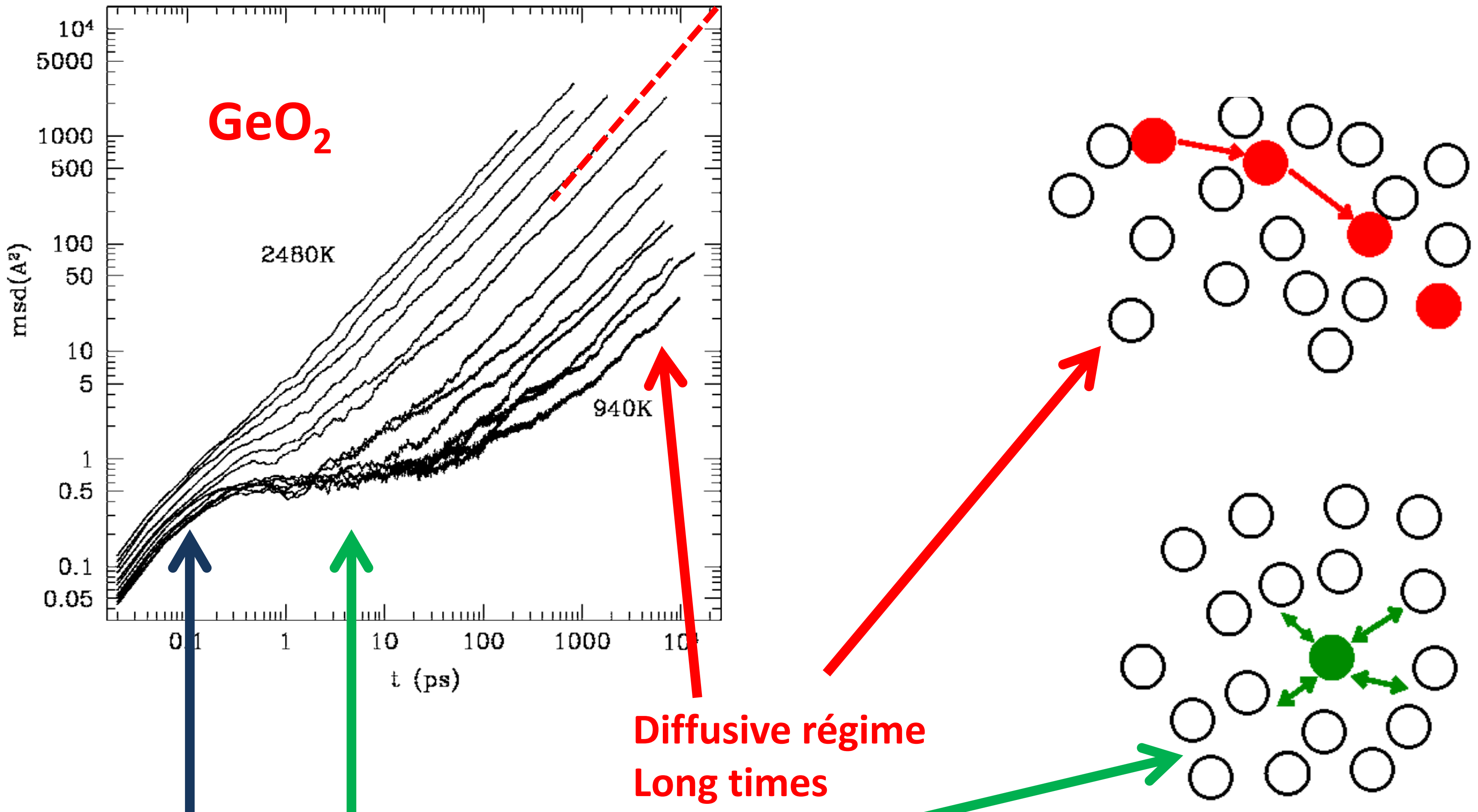
Bauchy et al., PRL 2013

A-B Lennard-Jones liquid



Kob PRE 2000

More insight into the msd…



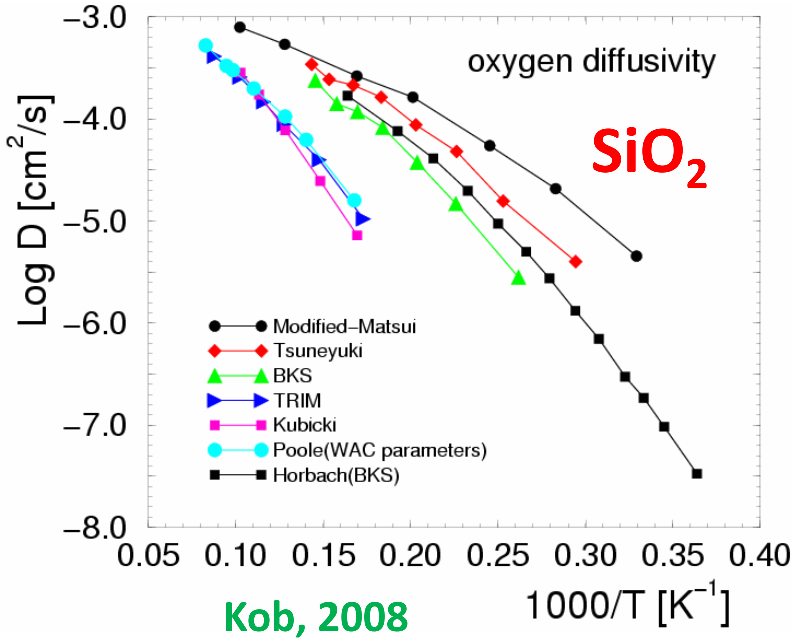
Diffusive régime
Long times

Ballistic régime
msd~t^2
Short time

Caging régime (LT)

Behavior with temperature

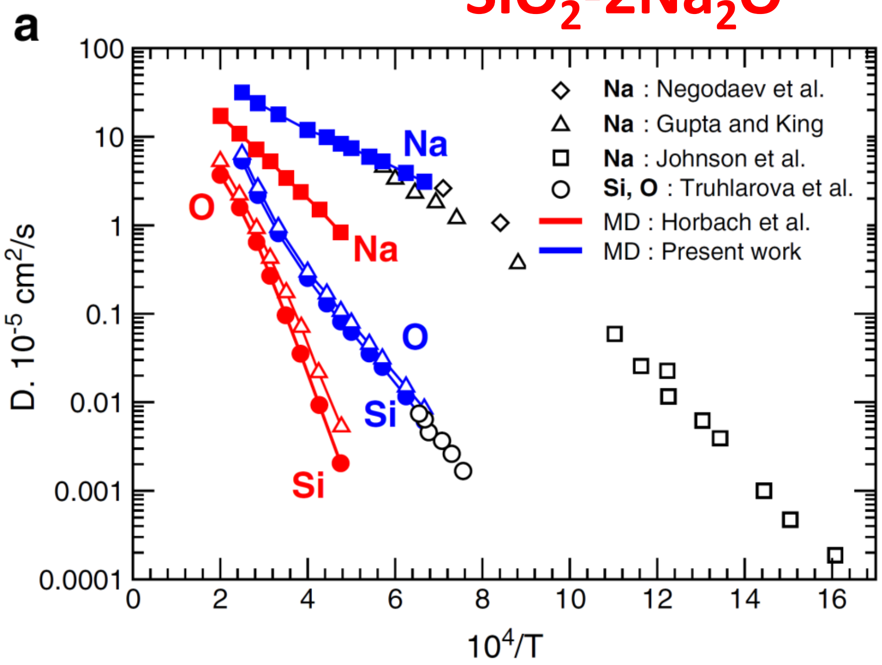
Usually, a gentle Arrhenius behavior :
$D=\exp[-E_A/k_BT]$



SiO_2

Kob, 2008

SiO_2-$2Na_2O$



Bauchy et al. Chem Geol. 2013

- Species dependent. Na diffuses faster than Si or O in silicates

Curvature linked with EOS

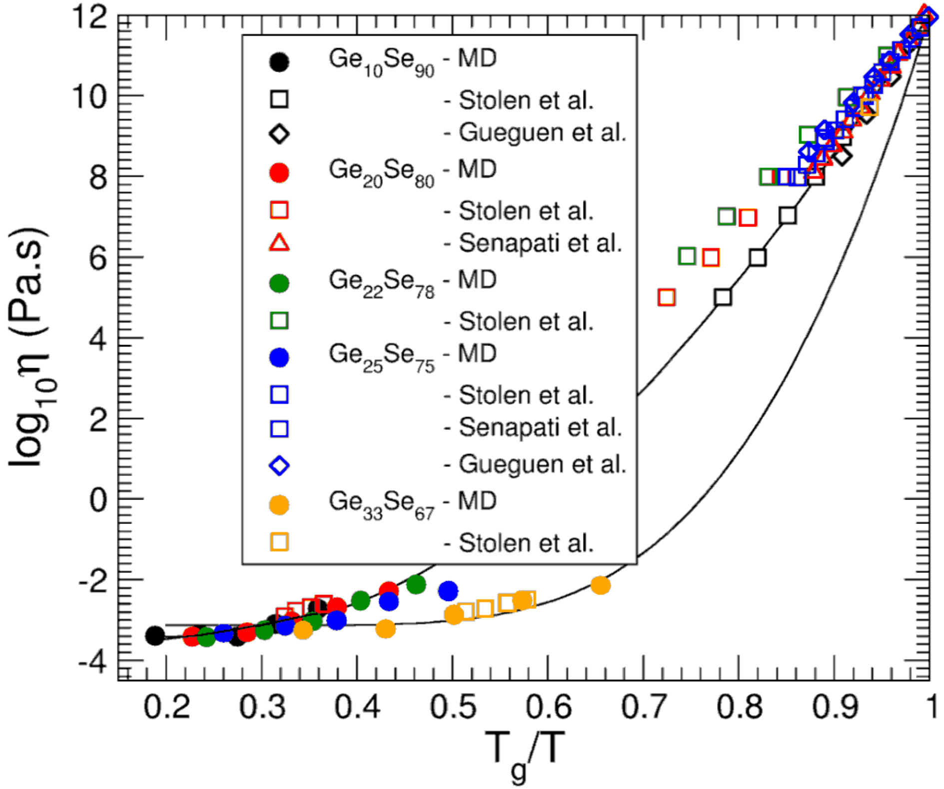
Agreement on structure does not reflect the quality of the potential. Dynamics !

Tentative connection with viscosity

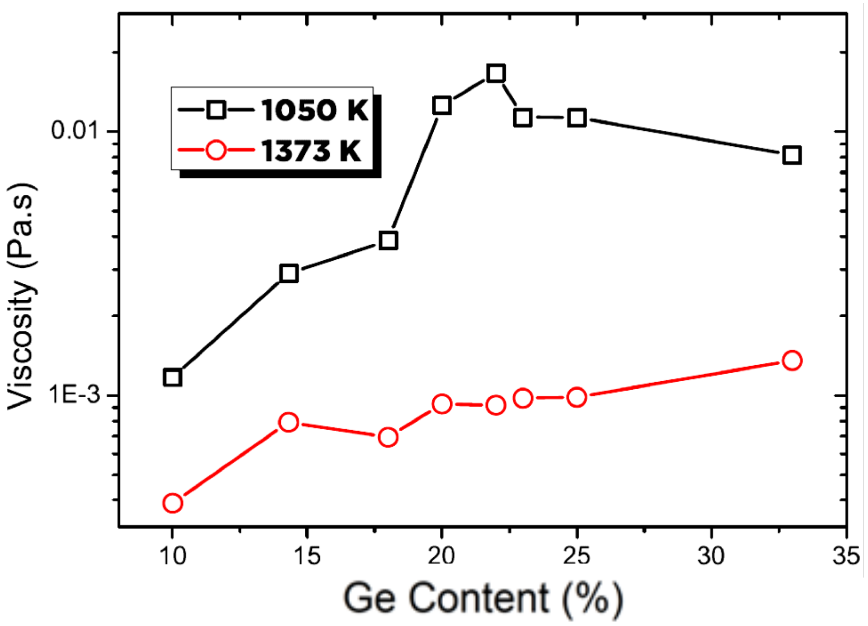
Calculating viscosity using Stokes-Einstein :

$$\eta = \frac{k_B T}{6\pi R D}$$

$$R = 0.5\rho^{-1/3}$$



Direct comparison for $Ge_{20}Se_{80}$ and $Ge_{33}Se_{66}$



Yildirim, Nature Comm. 2016

Clear decoupling between MD and experimental ranges

Behavior of the diffusion constant with other thermodynamic variables

- Dependence on V or P.
- Usually at fixed V (e.g. V_g) and P non-zero

H_2O

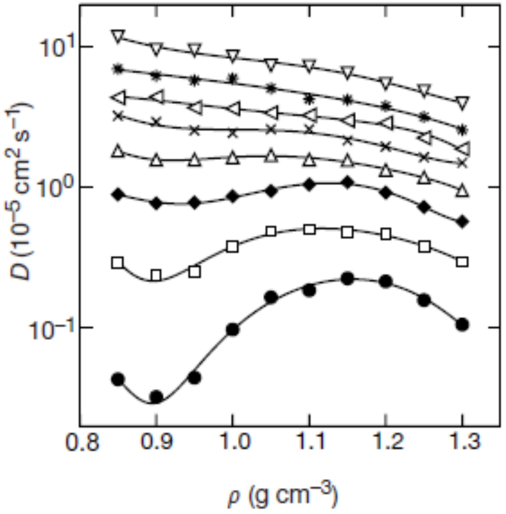
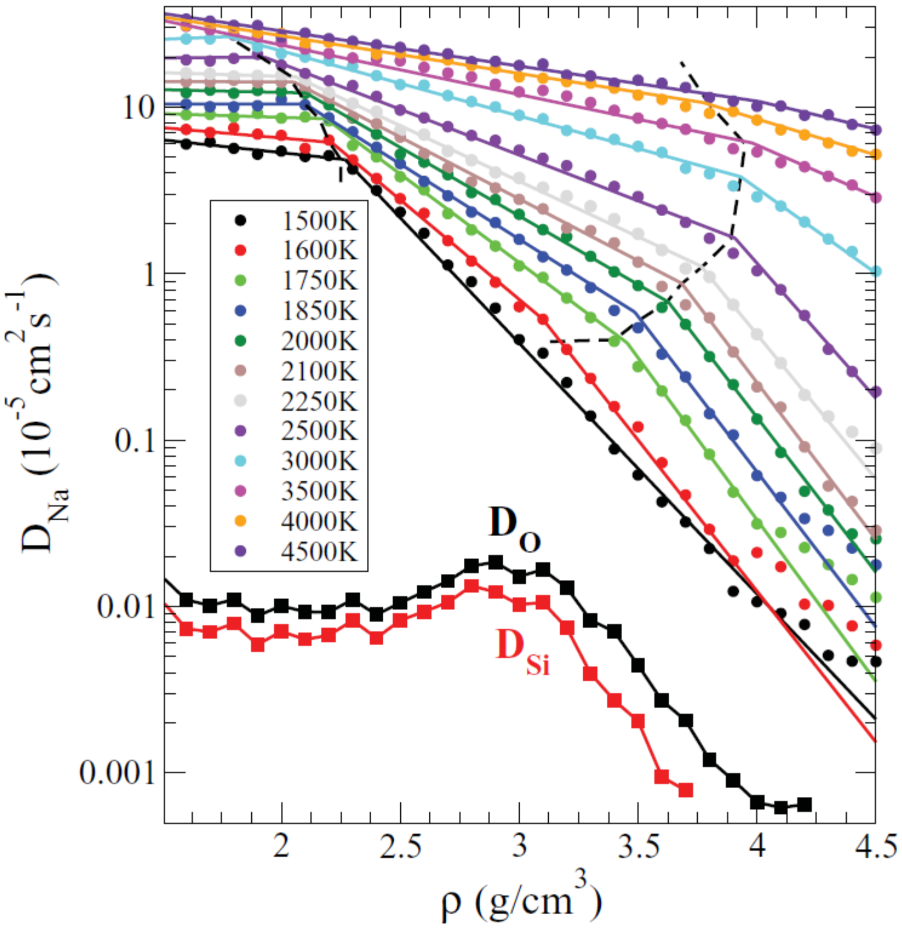
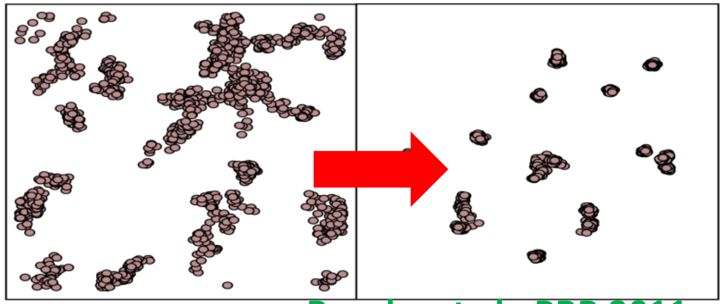


Figure 3 Density dependence of the diffusion coefficient, D, shown for eight isotherms. The curves from top to bottom correspond to temperatures T (in K) of: 400, 350, 320, 300, 280, 260, 240 and 220. The solid lines are fifth-order polynomial fits to the data, and are simply guides to the eye. The diffusion coefficient was calculated from the long-time behaviour of the mean squared displacement of the water molecules, $\langle r^2(t)\rangle$, using the Einstein relationship $6D = d\langle r^2(t)\rangle/dt$.

Errington et al. Nature 2001





Bauchy et al., PRB 2011

D) VAN HOVE CORRELATION FUNCTION

We first introduce a density correlation function G(**r**,**r'**,t) defined from the local atomic densities for a homogeneous system :

$$G(\mathbf{r},t) = \frac{1}{N}\langle\sum_{i=1}^{N}\sum_{j=1}^{N}\ \delta(\mathbf{r}-\mathbf{r}_i(t)+\mathbf{r}_j(0))\rangle$$

The Van Hove function is the probability density of finding a particle i in the vicinity of r at time t, knowing that a particle j is in the vicinity of the origin at time t=0.

We can split the function into two parts, **self and distinct**:

$$G_s(\mathbf{r},t) = \frac{1}{N}\langle\sum_{i=1}^{N}\delta((\mathbf{r}+\mathbf{r}_i(0)-\mathbf{r}_i(t))\rangle$$

Dirac at t=0

$$G_d(\mathbf{r},t) = \frac{1}{N}\langle\sum_{i\neq j}^{N}\delta(\mathbf{r}+\mathbf{r}_i(0)-\mathbf{r}_j(t))\rangle$$

g(r) at t=0

<u>Physical interpretation:</u>

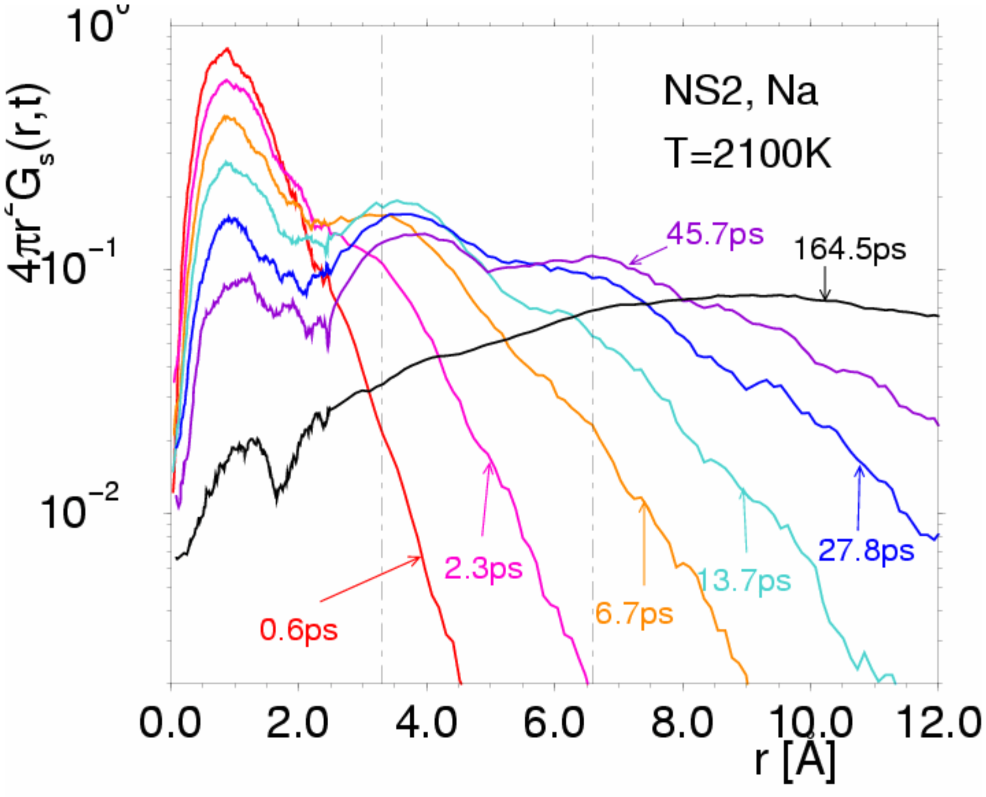
- The self part $G_s(r,t)$ is the probability density of finding a particle i at time t knowing that this particle was at the origin at time 0. Probability that a particle has moved a distance r in time t (dynamics).

$$G_s(\mathbf{r},t) = \frac{1}{N}\langle \sum_{i=1}^{N} \delta((\mathbf{r} + \mathbf{r}_i(0) - \mathbf{r}_i(t))\rangle$$

- The distinct part $G_d(r,t)$ is the probability density of finding a particle j different from i at time t knowing that the particle I was at the origin at time t=0. Probability to find at time t a different particle at a distance r from a place at which at time t=0 there was a particle. And $G_d(r,0)=g(r)$.

$$G_d(\mathbf{r},t) = \frac{1}{N}\langle \sum_{i\neq j}^{N} \delta(\mathbf{r} + \mathbf{r}_i(0) - \mathbf{r}_j(t))\rangle$$

Examples: Self part in Na silicates



Kob, PRB 2000

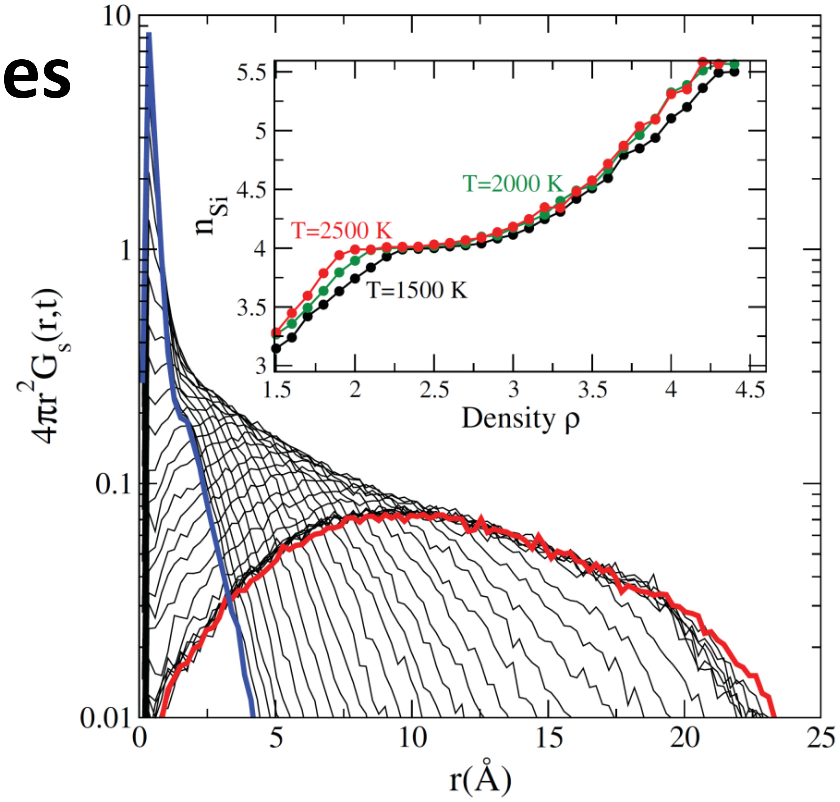


FIG. 4. (Color online) Van Hove function $G_s(r,t)$ of the NS3 system at 2000 K and fixed time $t = t_0 = 20$ ps for various densities between 2.0 and 4.5 g/cm^3. The red and blue curves correspond to 2.0 and 4.5 g/cm^3, respectively. The insert shows the change in Si coordination number n_{Si} as a function of density for three selected temperatures.

Bauchy, PRB 2011

- Small times: rattling and hopping motion on the length scale of nearest neighbors.
- Spatial extent of the motion is determined by thermodynamic conditions: T (viscous slowing down) or P (motion blocked by the high density).

E) INTERMEDIATE SCATTERING FUNCTION

Instead of considering correlations in space, one can perform a study in reciprocal space, i.e. in Fourier components.

- **The intermediate scattering function** is defined as the Fourier transform of the Van Hove function:

$$F(\mathbf{k},t) = \int d\mathbf{k} G(\mathbf{r},t) e^{-i\mathbf{k}.\mathbf{r}}$$

out of which, can be defined a self and a distinct part:

$$F_s(\mathbf{k},t) = \int d\mathbf{k} G_s(\mathbf{r},t) e^{-i\mathbf{k}\mathbf{r}}$$

$$F_d(\mathbf{k},t) = \int d\mathbf{k} G_d(\mathbf{r},t) e^{-i\mathbf{k}\mathbf{r}}$$

Instead of Fourier transform, these functions can be also directly computed from the atomic trajectories.

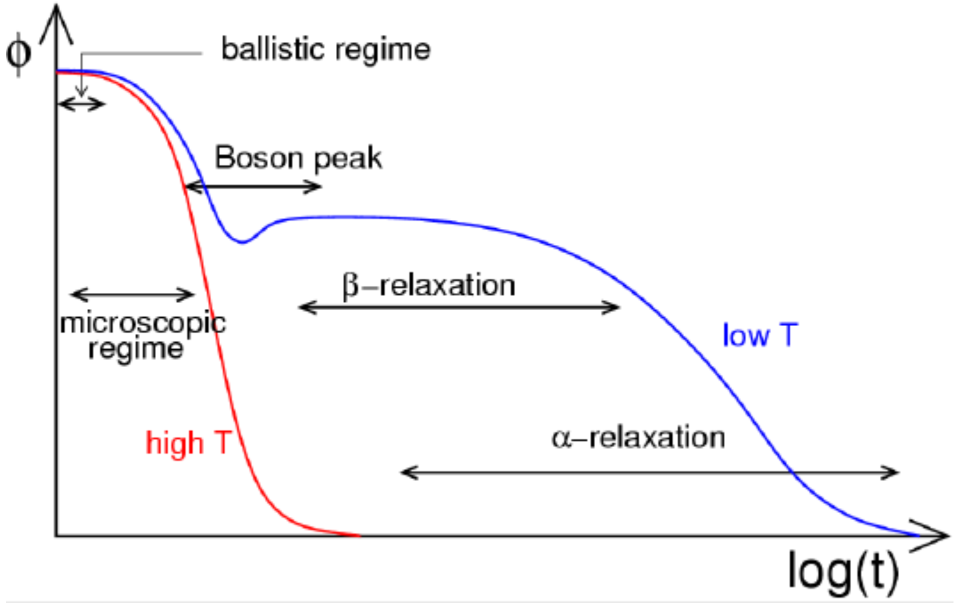
$$F_s(\boldsymbol{k},t) = \frac{1}{N}\left\langle \sum_{j=1}^{N} \exp[i\boldsymbol{k}.(\boldsymbol{r}_j(t) - \boldsymbol{r}_j(0)] \right\rangle$$

1. Self part (incoherent intermediate scattering function):

$$F_S(\boldsymbol{k},t)=\frac{1}{N}\left\langle\sum_{j=1}^{N}\exp[i\boldsymbol{k}.(\boldsymbol{r}_j(t)-\boldsymbol{r}_j(0)]\right\rangle$$

- F_s(k,t) can be directly compared to experiments from inelastic neutron or X-ray scattering.

- F_s(k,t) characterizes the mean relaxation time of the system (area under F_s(k,t) can be used to define a relaxation time). Spatial fluctuations of Fs(k,t) provides information on dynamic heterogeneities.



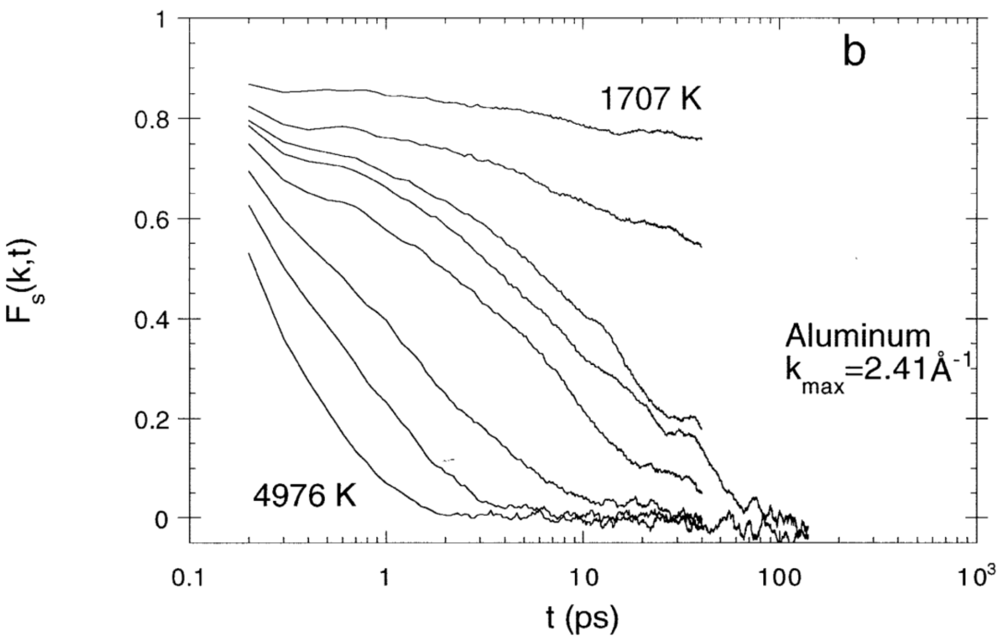
- **Short times :** balistic régime

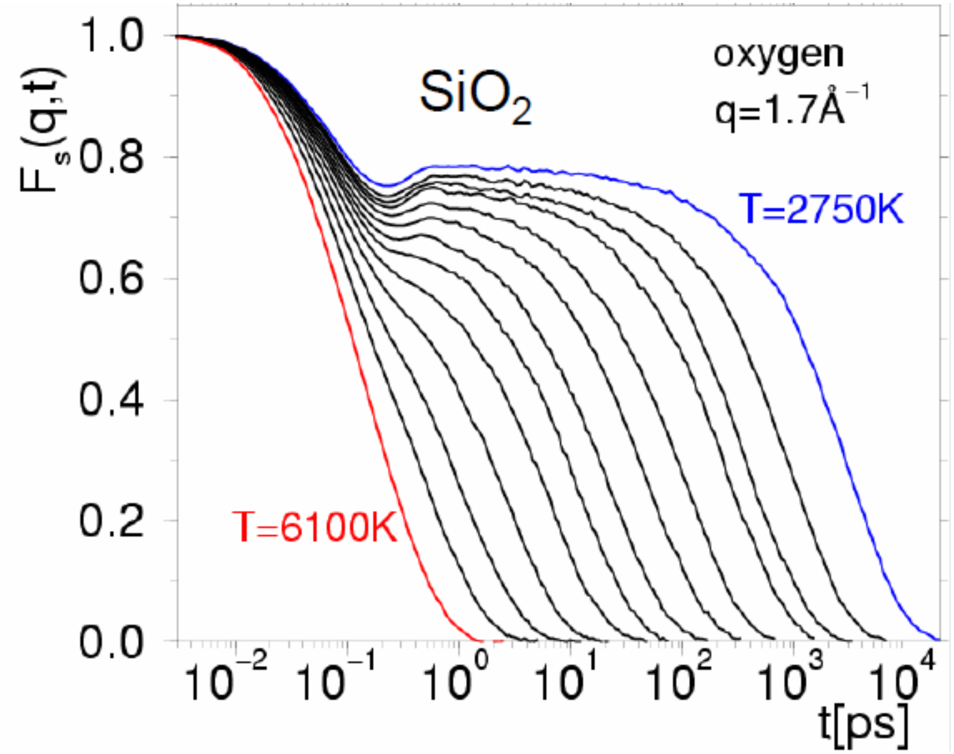
- **Intermediate times:** cage motion (β relaxation)

- **Long times:** Particles leaving cages. Kohlrausch (stretched exponential) behavior.

Examples :

$CaAl_2SiO_8$

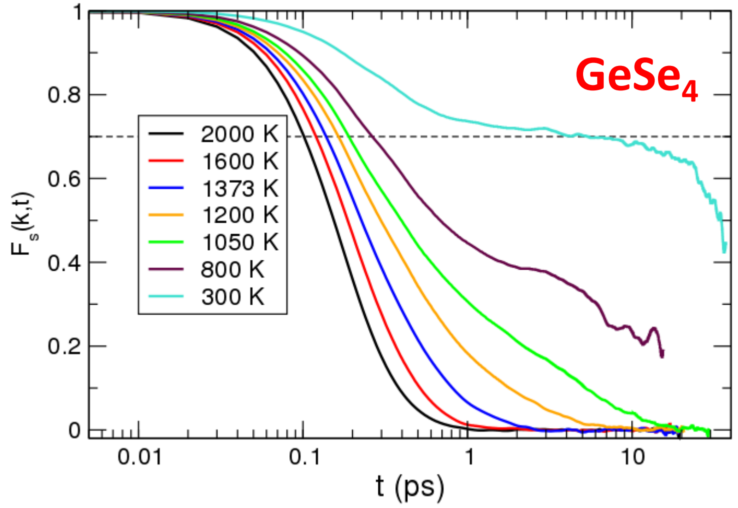




Morgan and Spera, GCA 2001

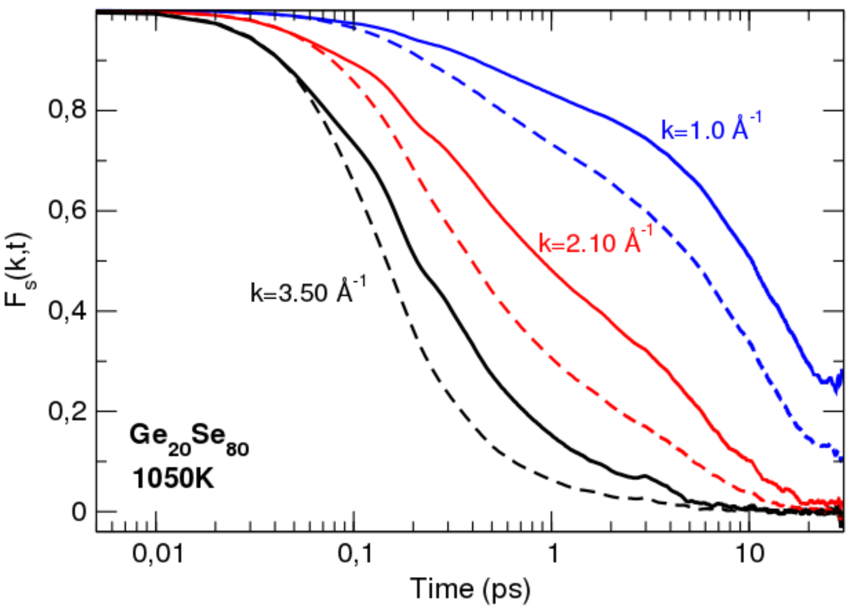
Cage motion (β régime) extends to long times at low T

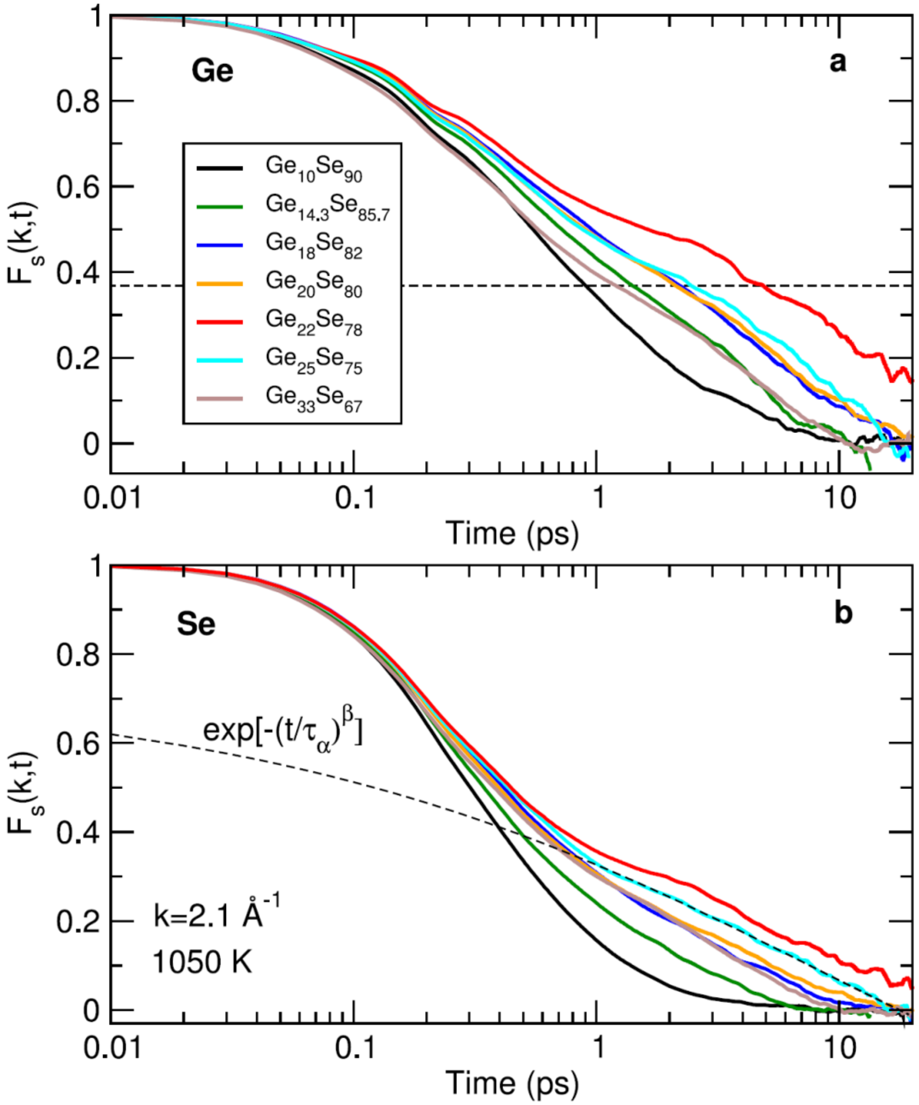
Horbach, Kob PRB 1999



Yildirim et al. JCP 2016

Examples (chalcogenides, Ge-Se) :





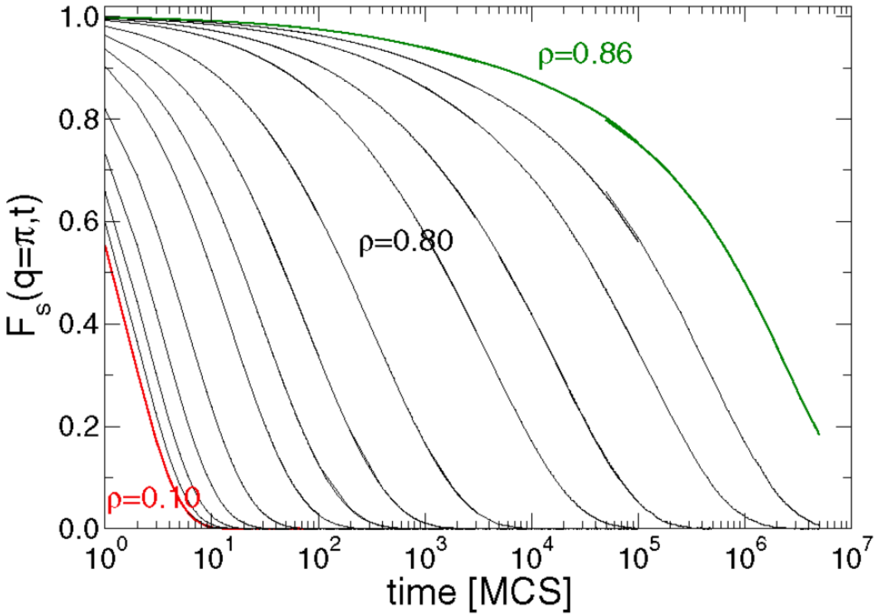
- Glassy relaxation at low k extends to longer times

- Kohlrausch fit at long times. Access to the relaxation time τ_α, β.

Slowing down of the dynamics: a more universal behavior…

MD simulation of hard spheres

Effet of density



Chaudhuri et al. AIP Conf. 2009

Experiments on bidimensional granular packing

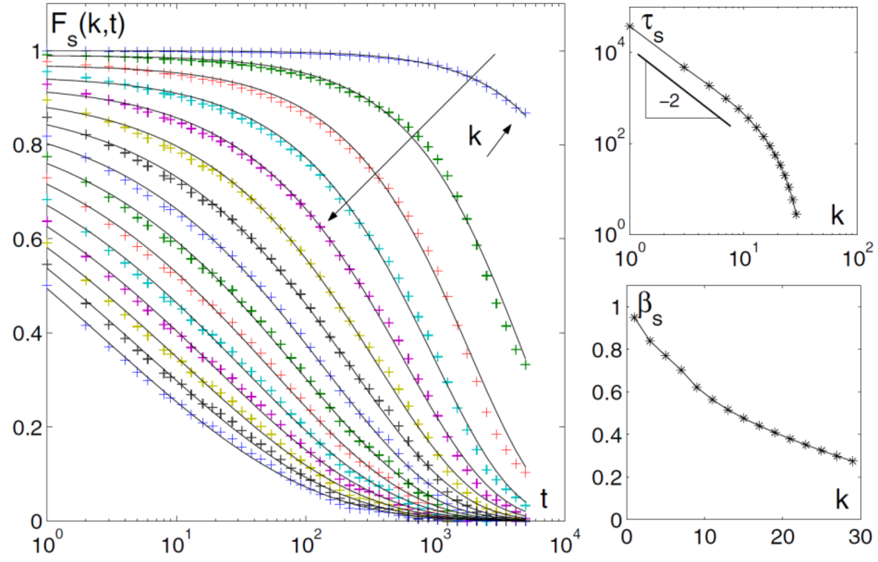


FIG. 1 (color online). On the left: $F_s(k, t)$ as a function of time for different odd values of the wave vector $k = 1, 3, \ldots, 29$ from top to bottom (as indicated by the arrow and the increasing $k \nearrow$). The black lines are fits of the form $\exp[-(t/\tau(k))^{\beta(k)}]$. On the right: $\tau(k)$ (top) and $\beta(k)$ (bottom) as a function of k.

Dauchot et al. PRL 2006

F) LINEAR RESPONSE THEORY

☐ Goal: Having MD generated trajectories at our disposal, we want to compute
- viscosity, electrical or thermal conductivity, mechanical properties, etc.

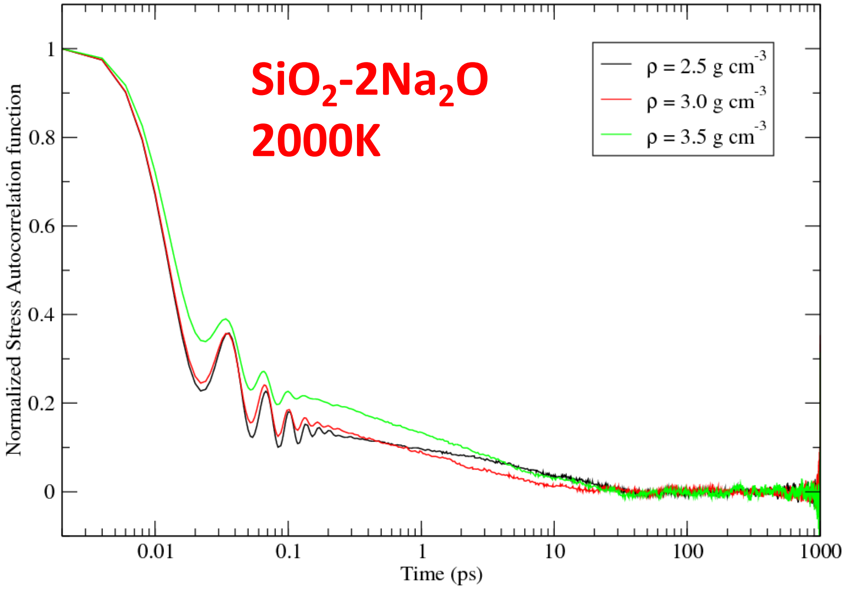
Use of linear response theory

☐ General idea (Onsager): Disturbance in a system created by a weak external perturbation decays in the same way as a spontaneous fluctuation in equilibrium.

☐ Linear response theory : link between time correlation functions and response to weak perturbations (Green-Kubo's fluctuation-dissipation relations)

$$\boxed{\sigma(t) = \frac{1}{Vk_BT}\int d\mathbf{r}d\mathbf{r}'\,\langle \mathbf{j}(\mathbf{r},0)\mathbf{j}(\mathbf{r}',t)\rangle}$$

$$\boxed{\eta = \frac{1}{Vk_BT}\int_0^\infty dt\,\langle \sigma_{xy}(0)\sigma_{xy}(t)\rangle}$$


SiO_2-$2Na_2O$
2000K

Example-1: Viscosity of a silicate liquid (NS2) and MORB under pressure

NPT (P=0), then NVE

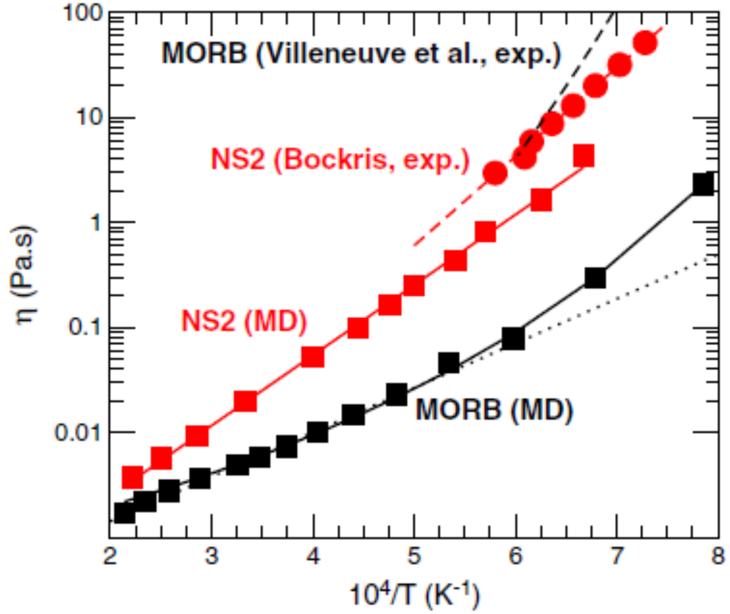
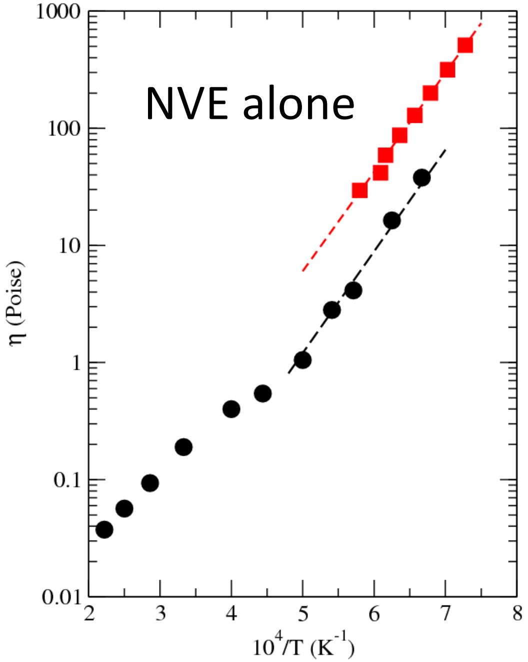
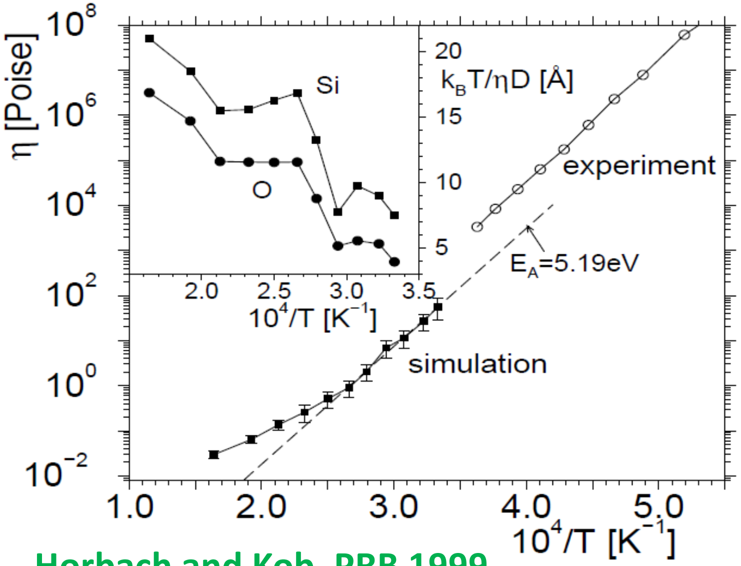


Fig. 3. Simulated viscosity of the NS2 liquid at zero pressure (filled red squares), compared to experimental data (red circles) from Bockris et al. (1955), together with simulated viscosity of the MORB liquid at zero pressure (filled black squares), compared to experimental data (broken black curve) from Villeneuve et al. (2008). The dotted line is a high temperature Arrhenius fit for the MORB data whereas the solid line is a TVF fit (see text for parameters).

Bauchy et al. Chem. Geol. 2013


NVE alone



Horbach and Kob, PRB 1999

Example-1: Viscosity of a silicate liquid (NS2) and MORB under pressure

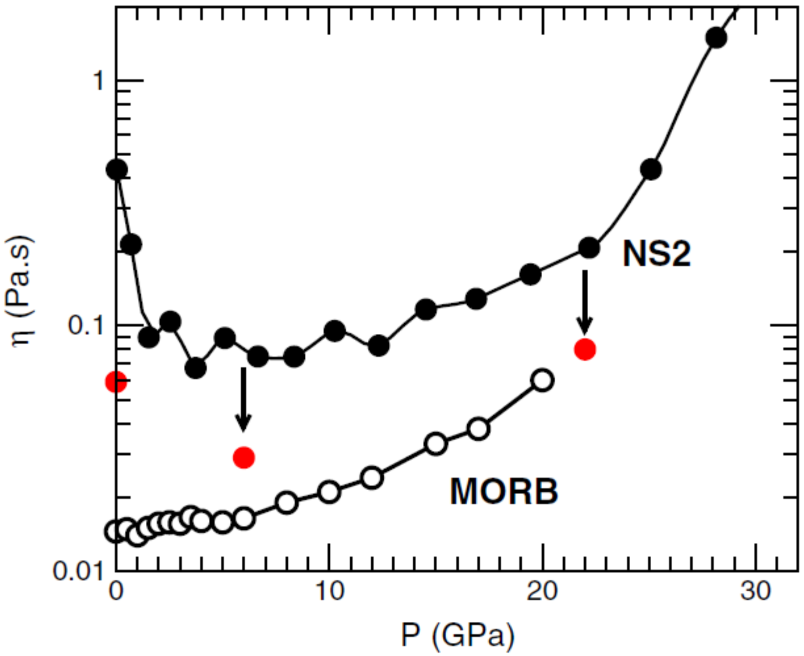


Fig. 6. Simulated viscosity of a NS2 liquid at T = 2000 K (filled circles) and a MORB liquid at T = 2273 K (open circles) as a function of pressure. Red circles correspond to the simulated viscosity of three selected densified NS2 using the potential of Guillot and Sator (2007a).

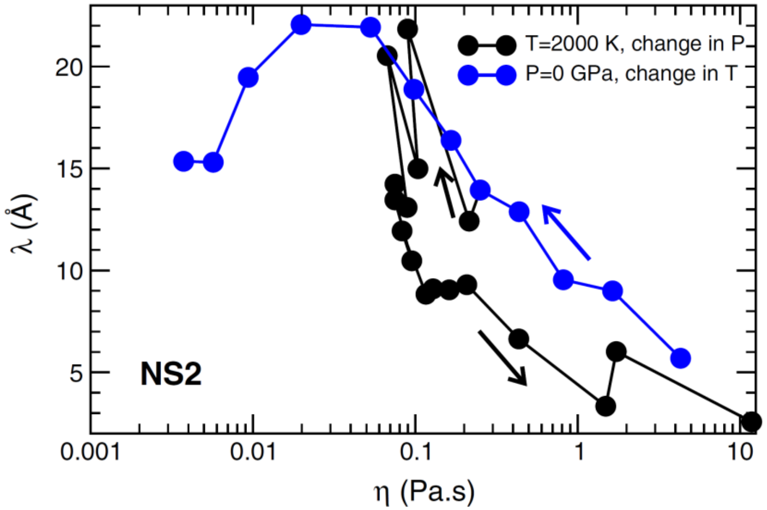
☐ Detecting anomalies (minima in viscosity)

☐ Checking for empirical relationships

Eyring (1948): $\boldsymbol{\eta = k_B T/\lambda D}$

With λ a jump distance ($d_{O\text{-}O}$~ a few A)

- Compute (MD) D and η
- Valid only at high viscosity



Beyond linear response theory - usefulness of MD

- Channel conduction in silicates

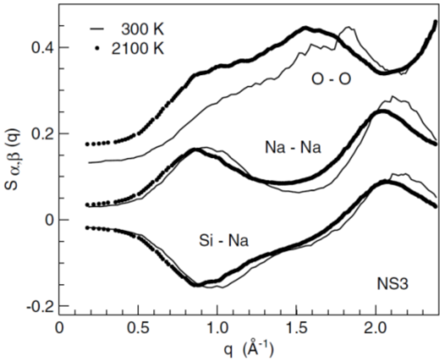
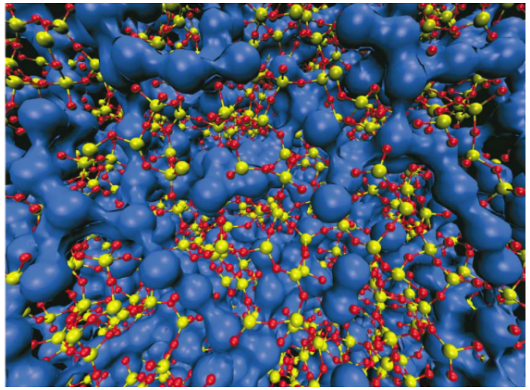


FIG. 3. Partial structure factors $S_{O,O}(q)$, $S_{Na,Na}(q)$, $S_{Si,Na}(q)$ as obtained by the simulation in glassy and liquid sodium trisilicate at experimental densities. $S_{O,O}(q) + 0.1$ for clarity.



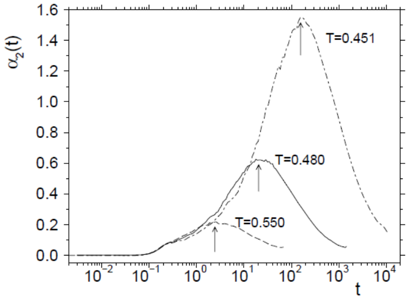
Meyer et al. PRL 2004

- Energy landscapes

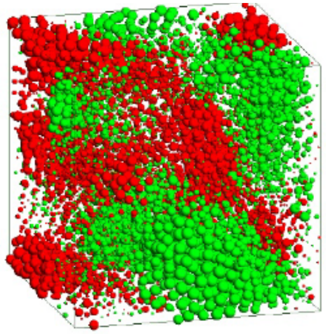
Sciortino et al. PRL 2002

- Non-Gaussian parameter

Kob et al. PRL 1997

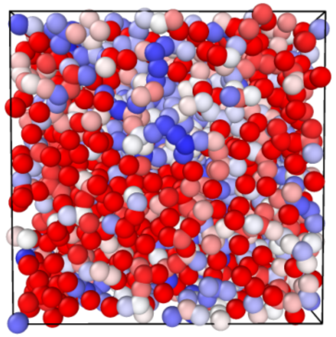


- Isoconfigurational Ensemble



Matharoo et al. PRE 2006

- Dynamic heterogeneities



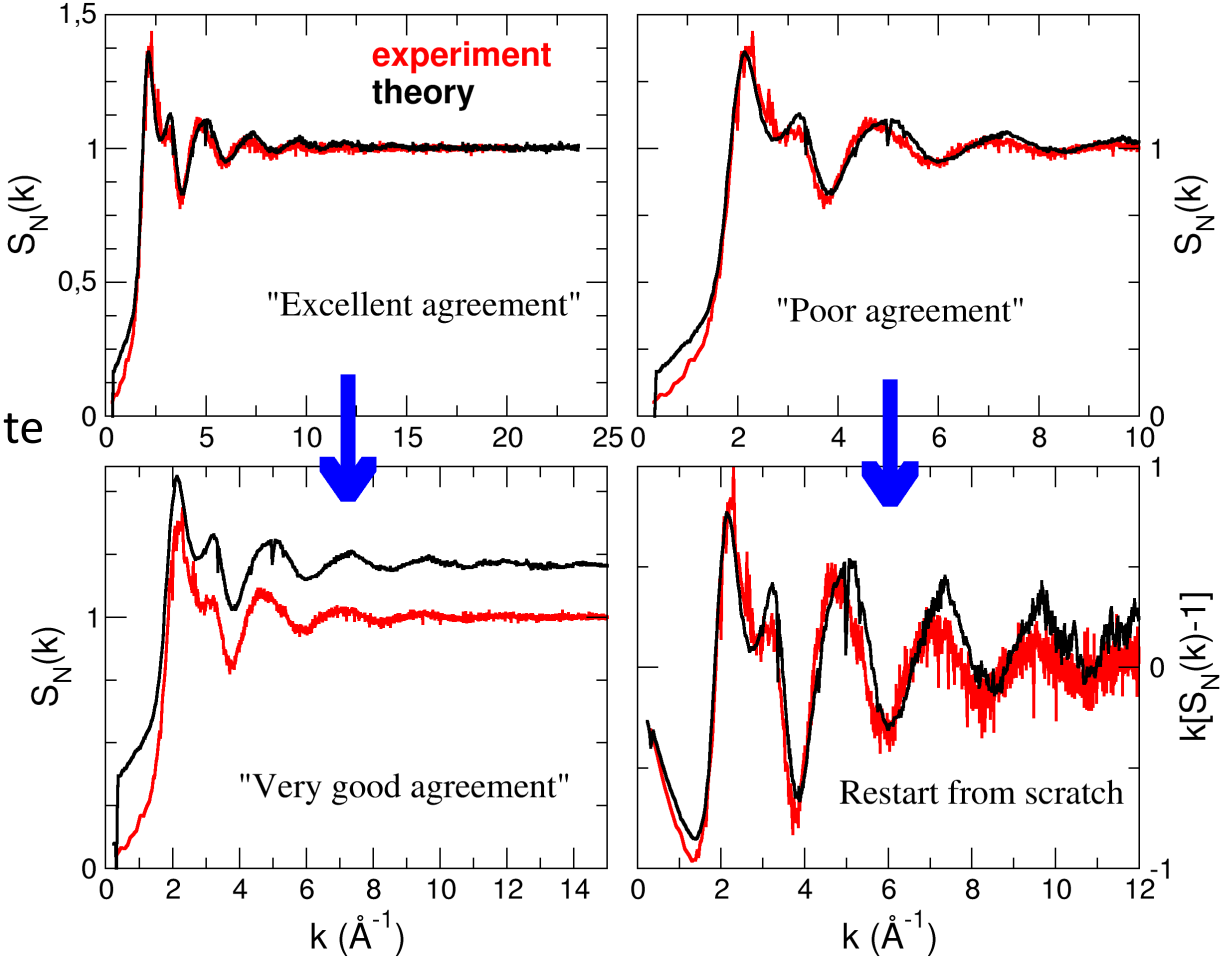
Berthier et al. (Book 2017)

Conclusion:

- ☐ Dynamics of glass-forming systems can be followed with numerous tools using computer simulations.
- ☐ Insight into structure and link between structure and dynamics.
- ☐ Functions quantify the slowing down of the dynamics.

Final recommendation regarding structural properties

1. Do the best you can.
2. Don’t fool the reader.
3. Be honest with the data
4. Do not attempt to dissimulate
5. Unique S(k) ?



Uncarefully simulated liquid $GeTe_4$