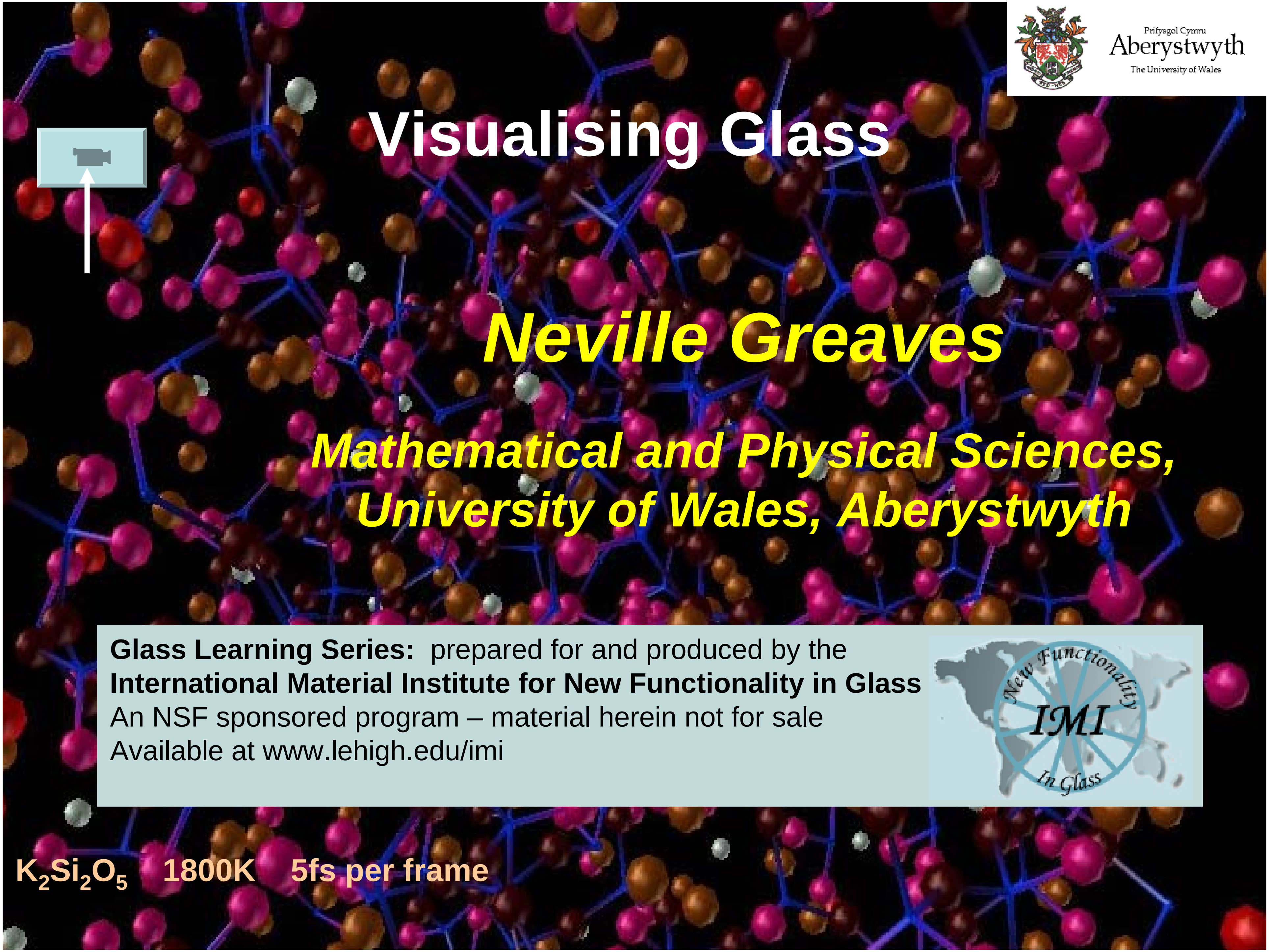

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Visualising Glass

Neville Greaves

Mathematical and Physical Sciences, University of Wales, Aberystwyth

Glass Learning Series: prepared for and produced by the
International Material Institute for New Functionality in Glass
An NSF sponsored program – material herein not for sale
Available at www.lehigh.edu/imi

New Functionality In Glass IMI

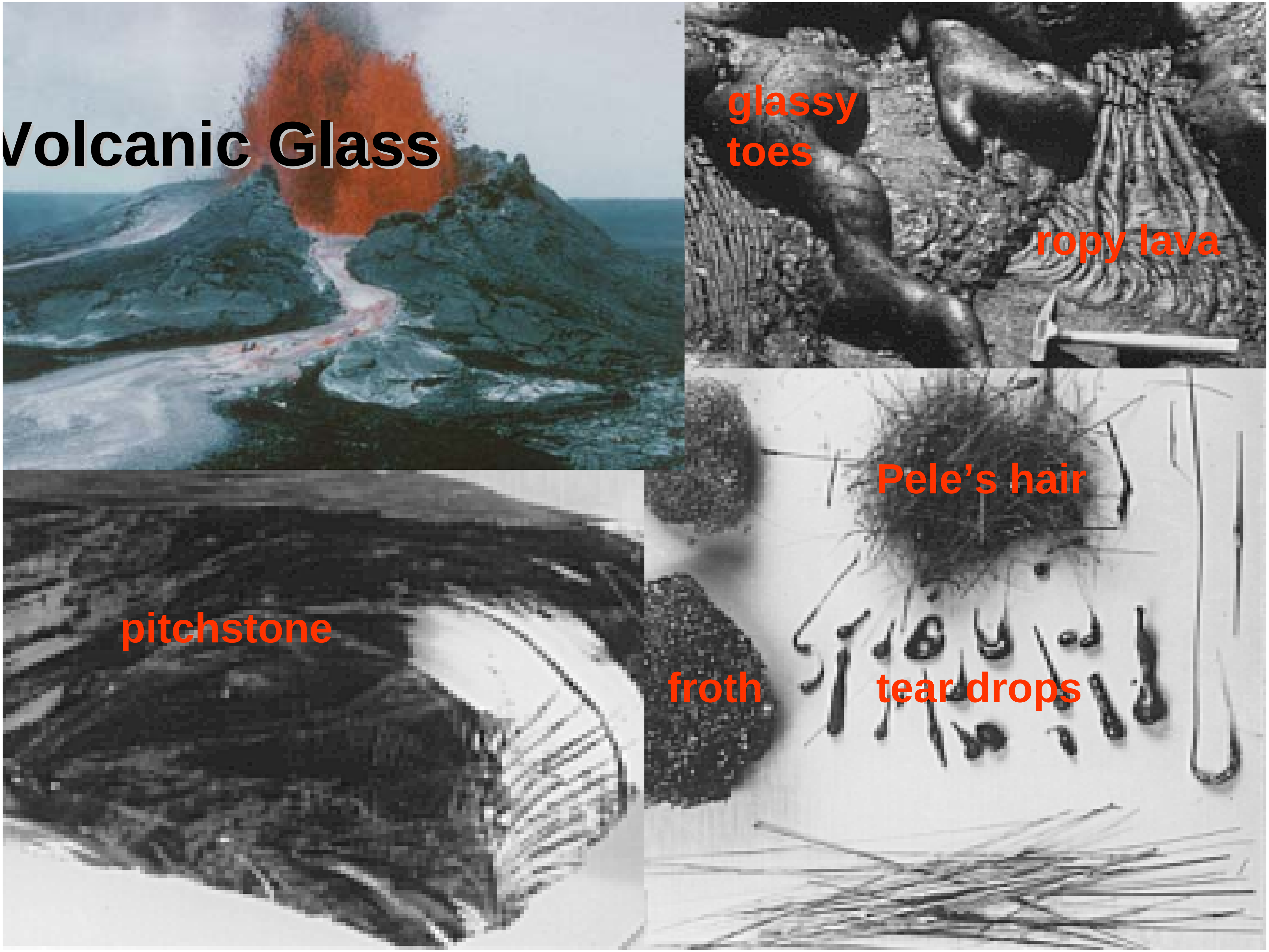
$K_2Si_2O_5$ 1800K 5fs per frame


history
glass
formation
visualisation
glass transition
computer
simulation
glass structure
Patrick Reyntiens - Homage to Hector Bérlioz
© Photograph provided courtesy of Patrick Reyntiens

History

Very rapid quench = natural glass

Volcanic Glass



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History

If you want to produce zaginduru-coloured glass, you grind, separately, ten minas of immanakku-stone, fifteen minas of naga-plant ashes (and) 1 2/3 minas of “White Plant”. You mix (these) together. You put (them) into a cold kiln which has four openings (literally eyes) and arrange (the mixture) between the openings. You keep a good smokeless fire burning until the “metal” (molten glass) becomes fritted. You take it out and allow it to cool off. You grind it finely again. You collect in a clean dabtu-pan. You put into a cold chamber kiln. You keep a good smokeless fire burning until it glows golden yellow. You pour it into a kiln-fired brick and this is called (zuku-glass).

Assyrian recipe 3500 BC

History

"……with great wonder I observe that fire is almost everywhere the active agent. Fire takes in sand and gives back, now glass, now silver … now lead, now pigments, now medicines……"

Pliny, *Natural History* (68AD) p. xxxvi

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History

the Romans invented glass blowing between 1 BC and 1 AD

– also dichroic glass

Lycurgus Cup

History

the Venetians learned to fashion and decorate glass – starting around the Renaissance

Venetian filigrana tazza 16th – 17th century

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History

flat glass manufacture was perfected in Britain

opening of the Great Exhibition 1st may 1851 in the Crystal Palace by Queen Victoria

D Winfield

History – Glass Sculpture

Dale Chuhuly – *Venturi Window* at the Seattle Art Museum.

Glass Formation

Glass Formation

network

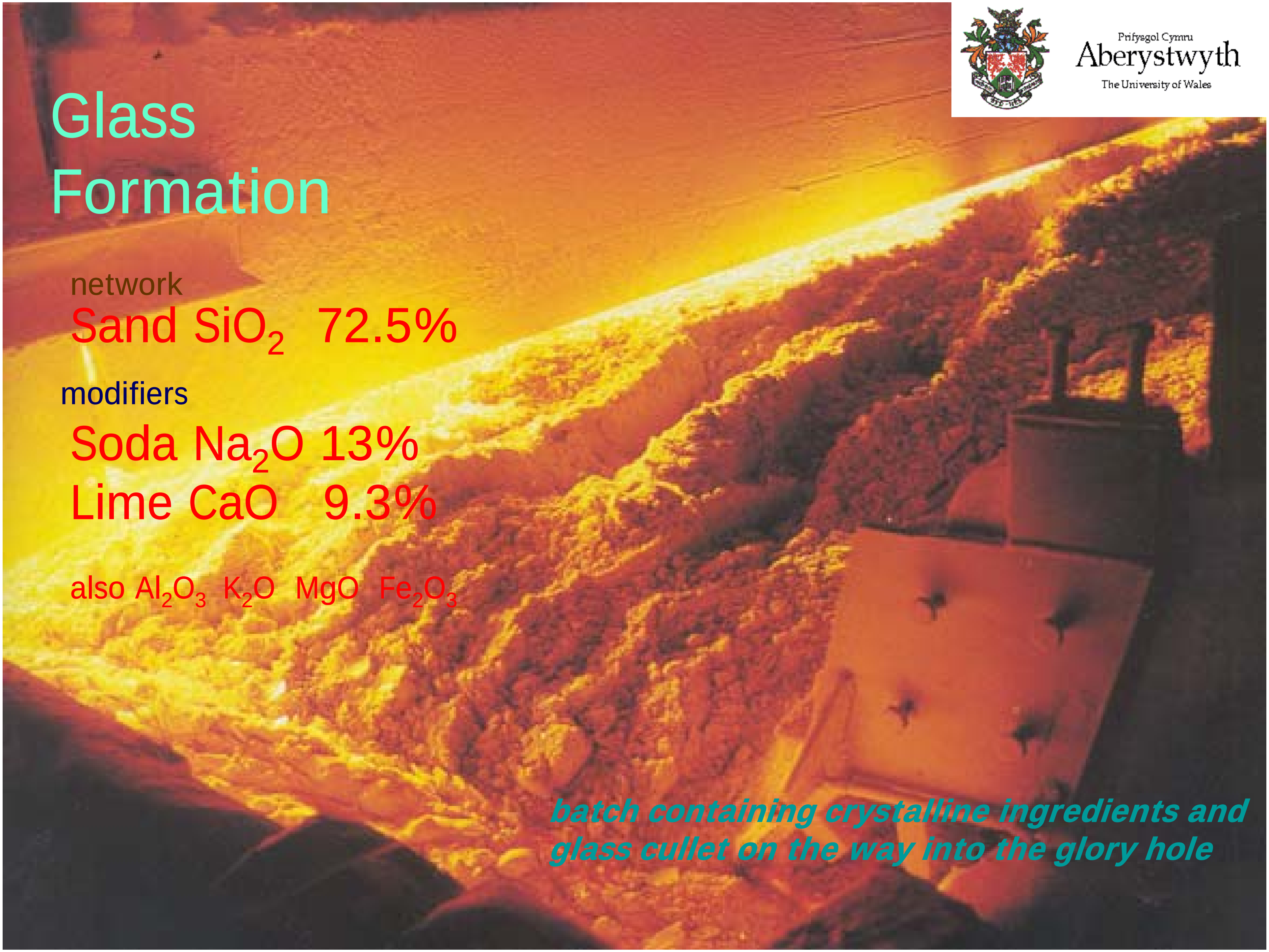
Sand SiO_2 72.5%

modifiers

Soda Na_2O 13%

Lime CaO 9.3%

also Al_2O_3 K_2O MgO Fe_2O_3



batch containing crystalline ingredients and glass cullet on the way into the glory hole

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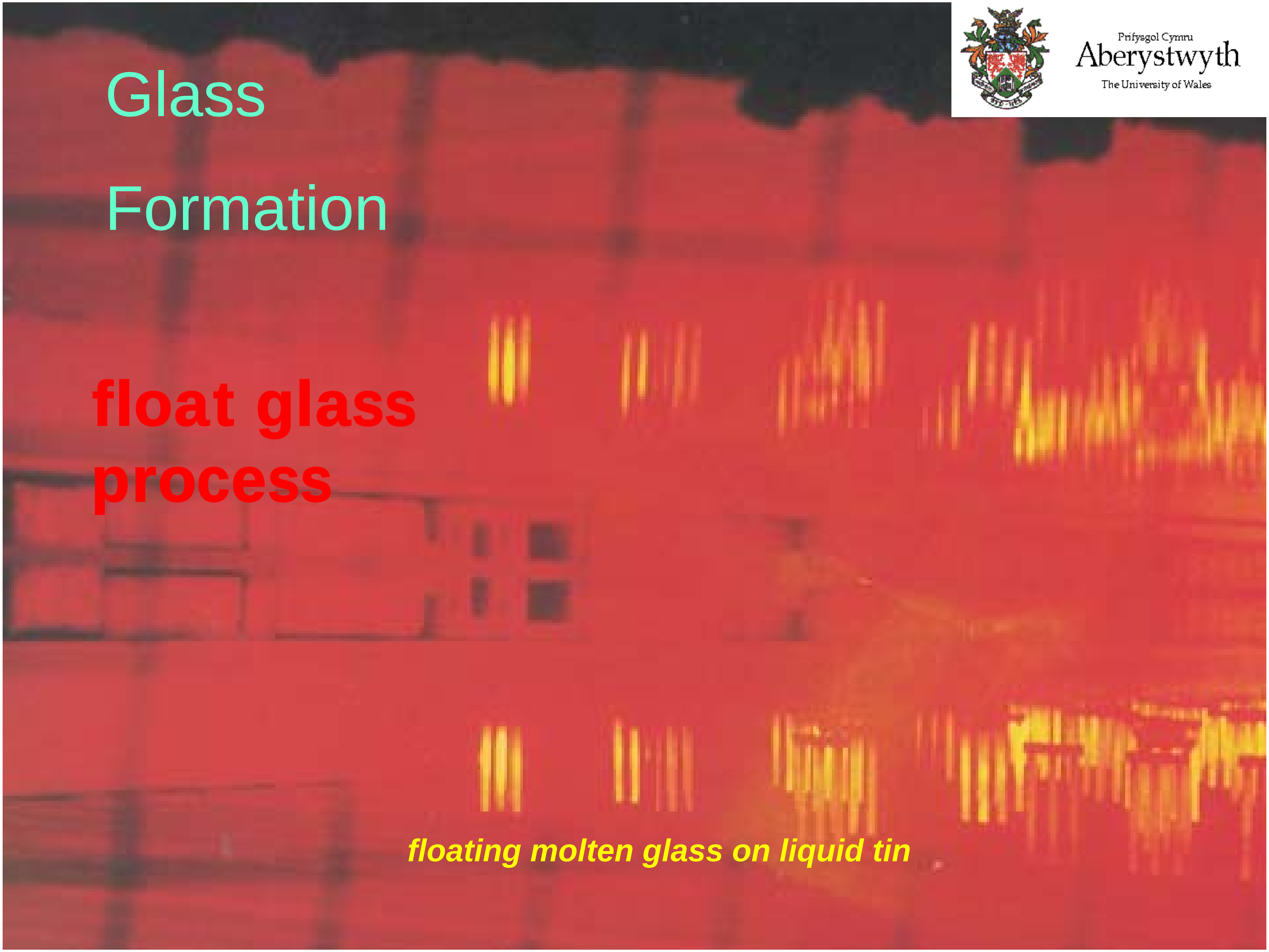
Glass

Formation

float glass process



floating molten glass on liquid tin

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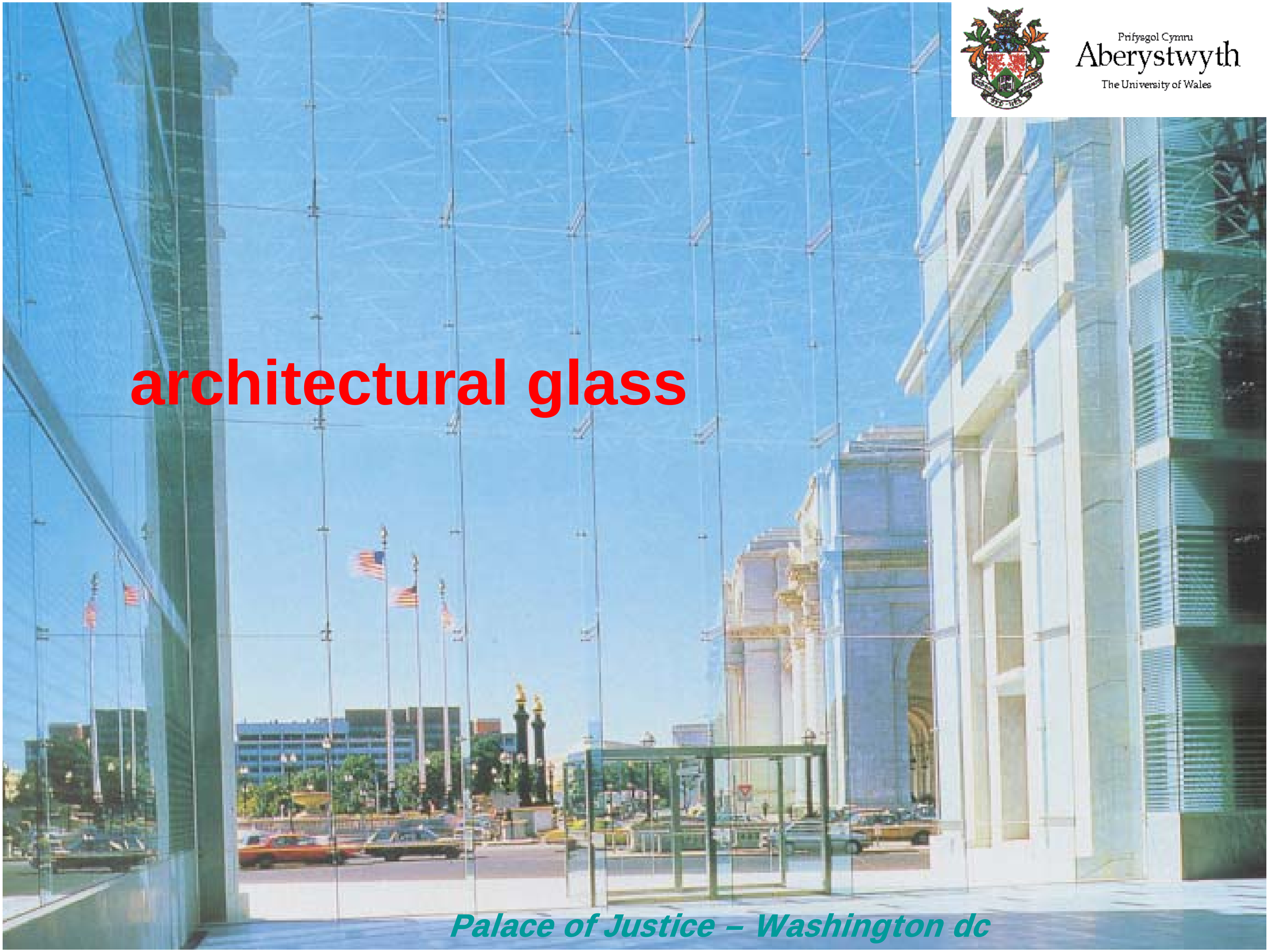
architectural glass

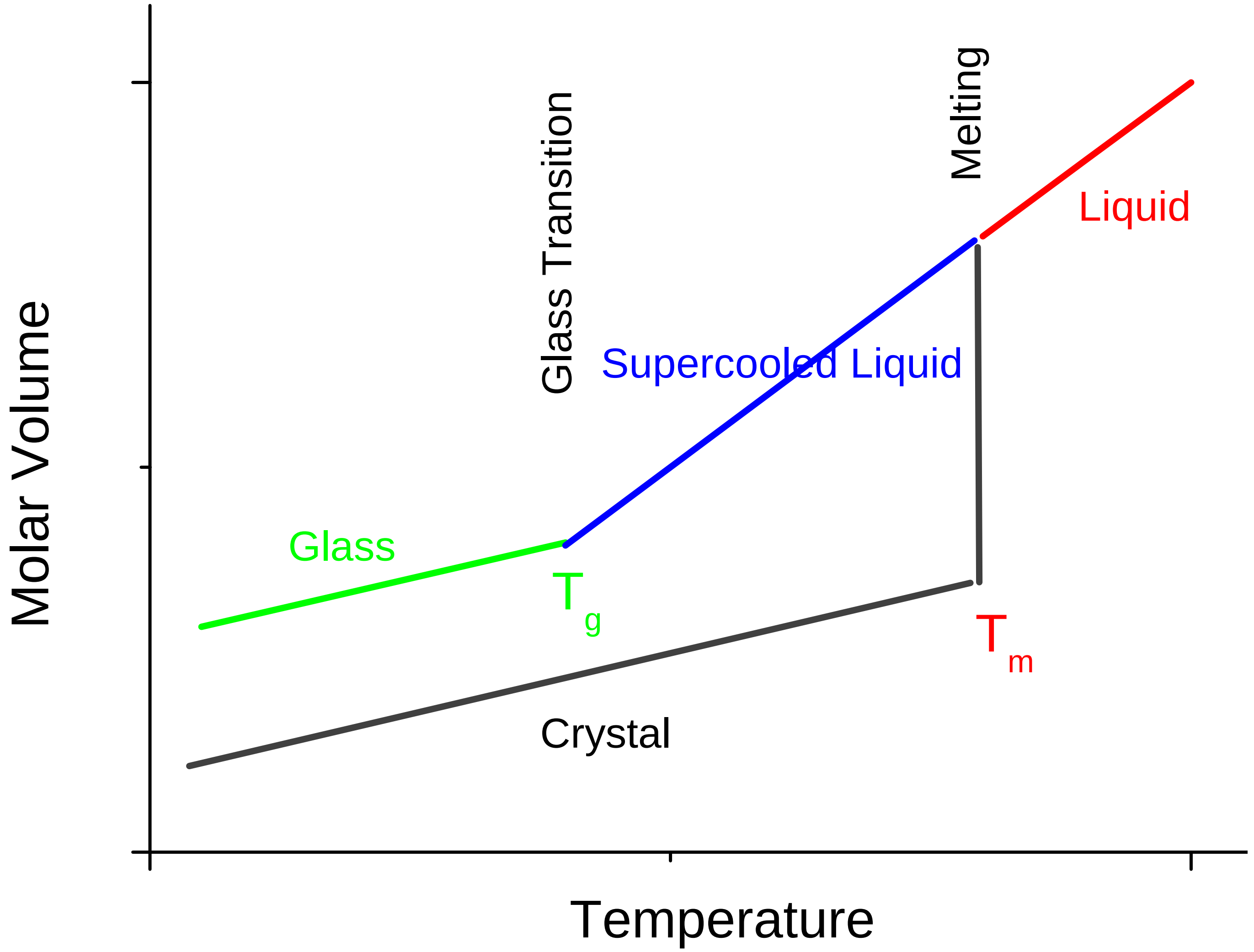


Palace of Justice – Washington dc

Glass Formation

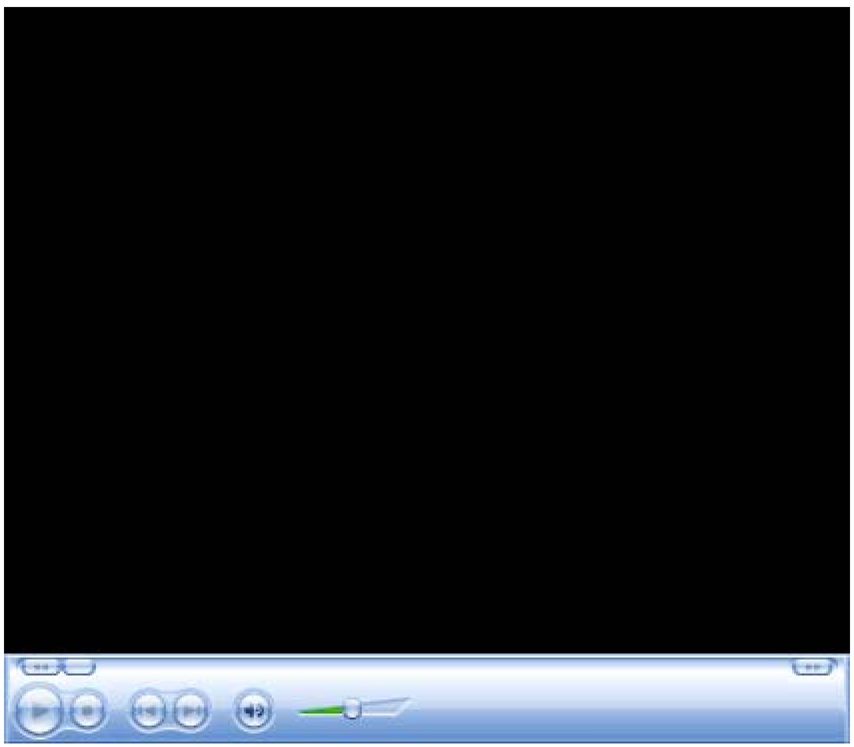
Glass Transition

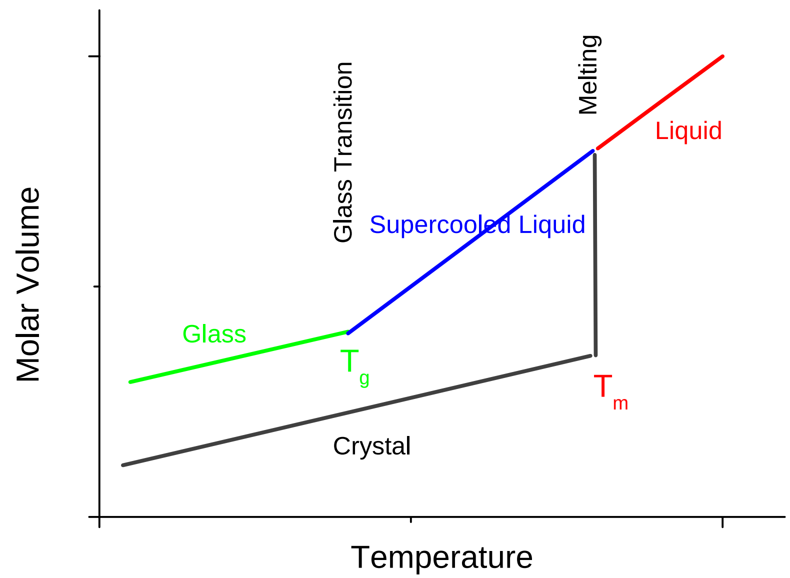
temperature below which viscosity is too great for crystallisation to occur



SAMPLE FOUNDARY

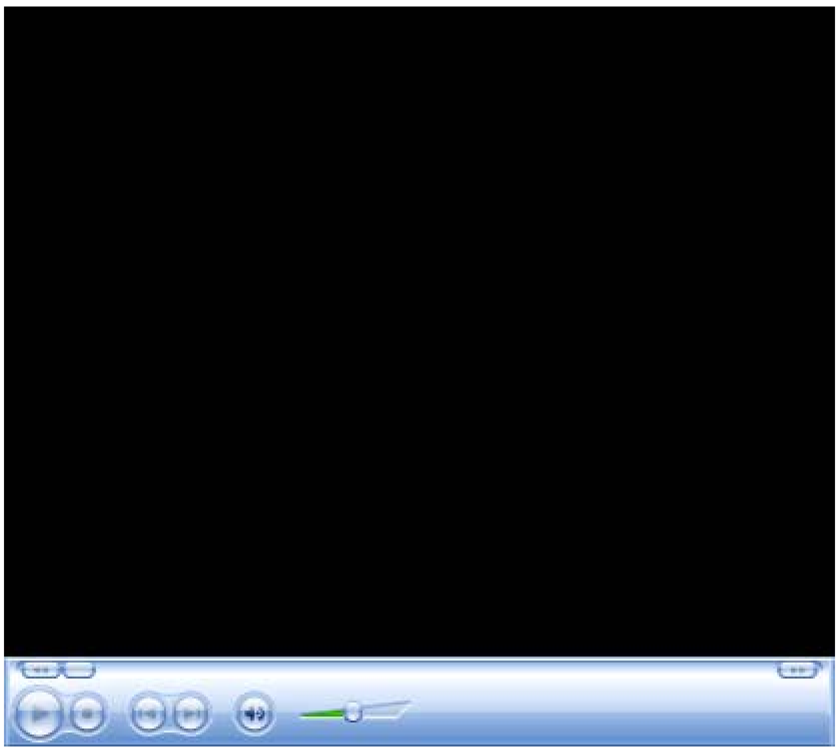
Preparation of a YA20 glass y melting three glass pieces to ~2000°C and cooling

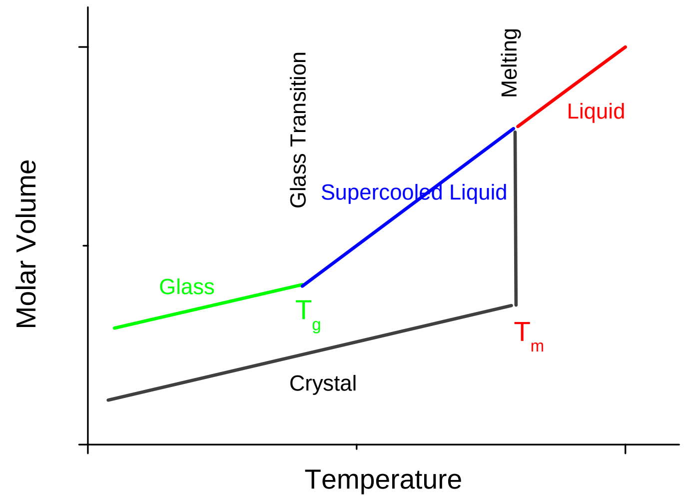


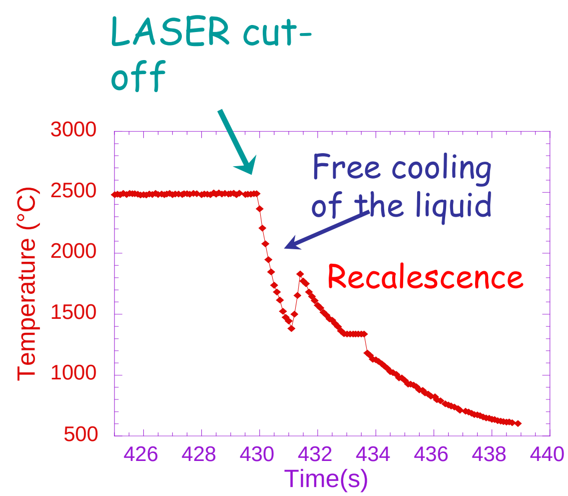


SAMPLE FOUNDARY

Preparation of crsytalline Al_2O_3 from melt at 2500°C







Shear in Solids and Liquids

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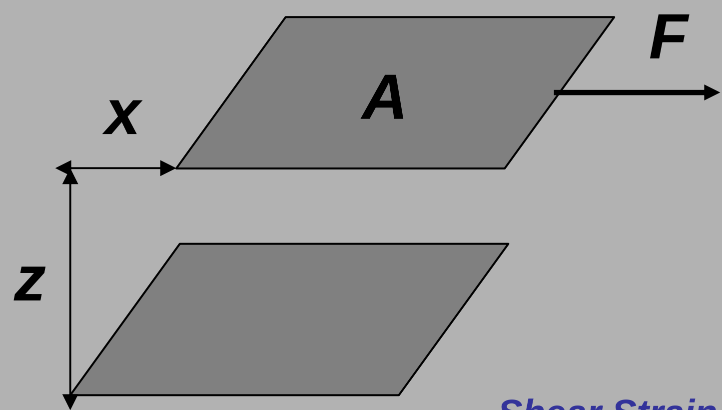
Elastic Shear



Shear Strain

$$\gamma = \frac{x}{z}$$

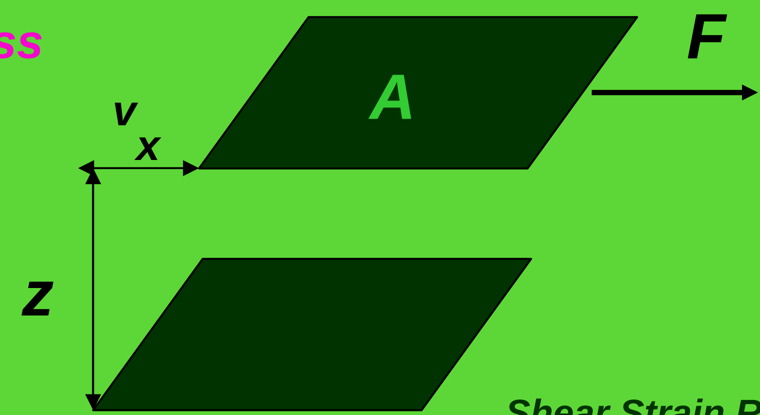
$$\sigma = G\gamma$$

G, Shear Modulus

Shear Stress

$$\sigma = \frac{F}{A}$$

Newton's Law of Viscosity



Shear Strain Rate

$$\frac{d\gamma}{dt} = \frac{v_x}{z}$$

$$\sigma = \eta \frac{d\gamma}{dt}$$

η, Viscosity

$$\sigma = G_{HF}\gamma$$

$$x = v_x \tau$$

G_{HF}, High Frequency Modulus

τ, Structural Relaxation Time

$$\sigma = G_{HF}\tau \frac{d\gamma}{dt}$$

$$\eta = G_{HF}\tau$$

Maxwell's Viscosity Equation

22 Decades of Viscosity

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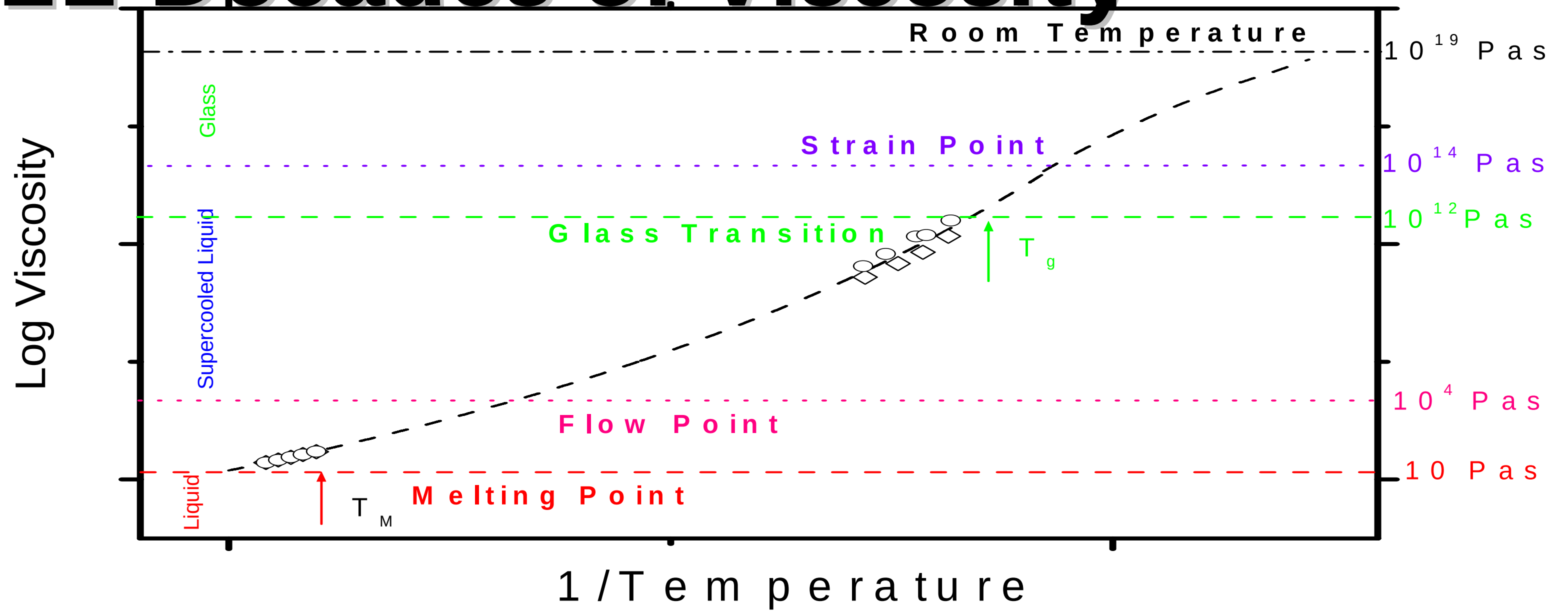
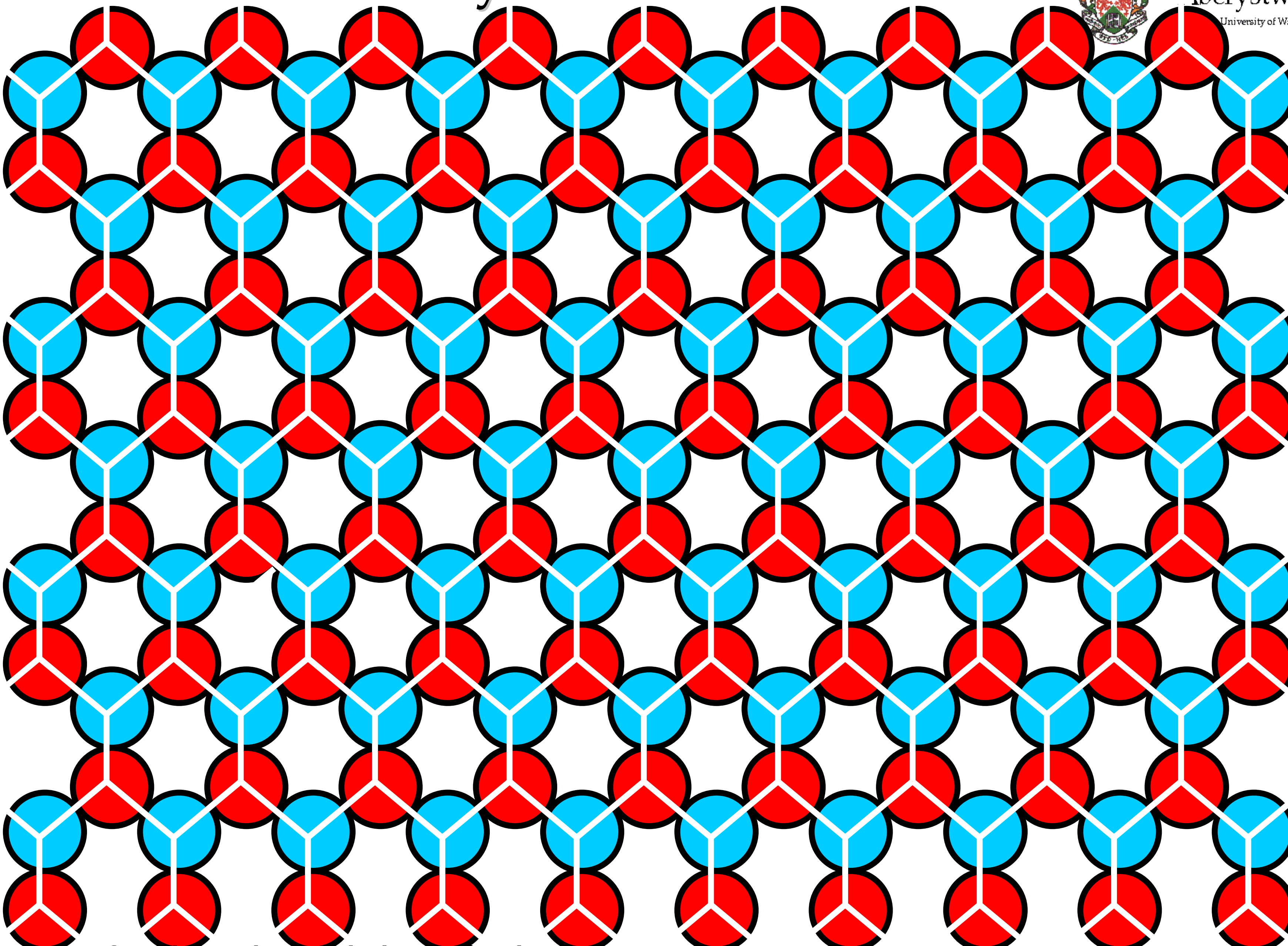
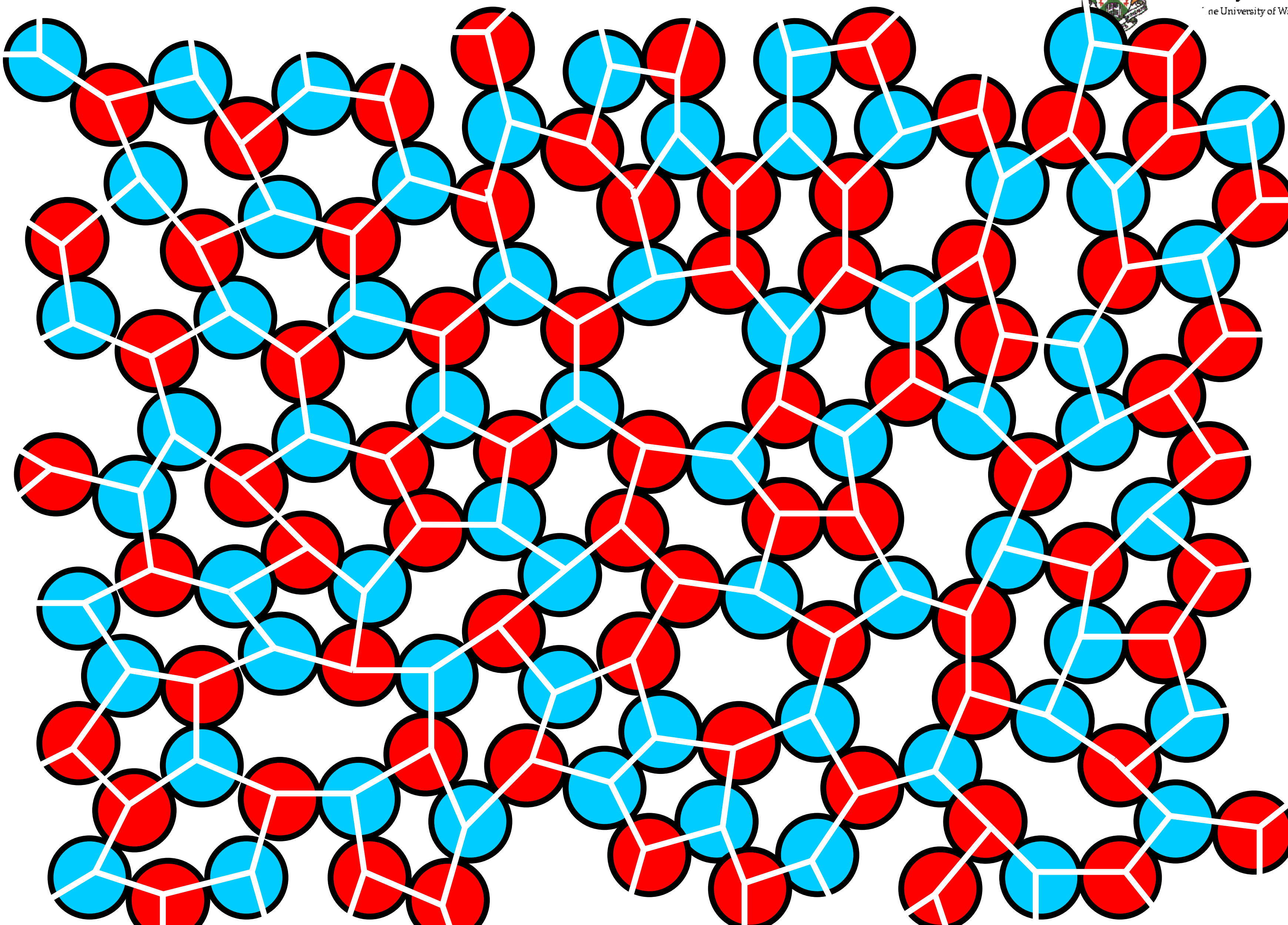


Water at 0°C → → $2\ 10^{-3}$ Pas

Crystalline Network



Continuous Random Network



Atomic Structure and Dynamics of Glass

Modelling the Atomic Structure of Glass

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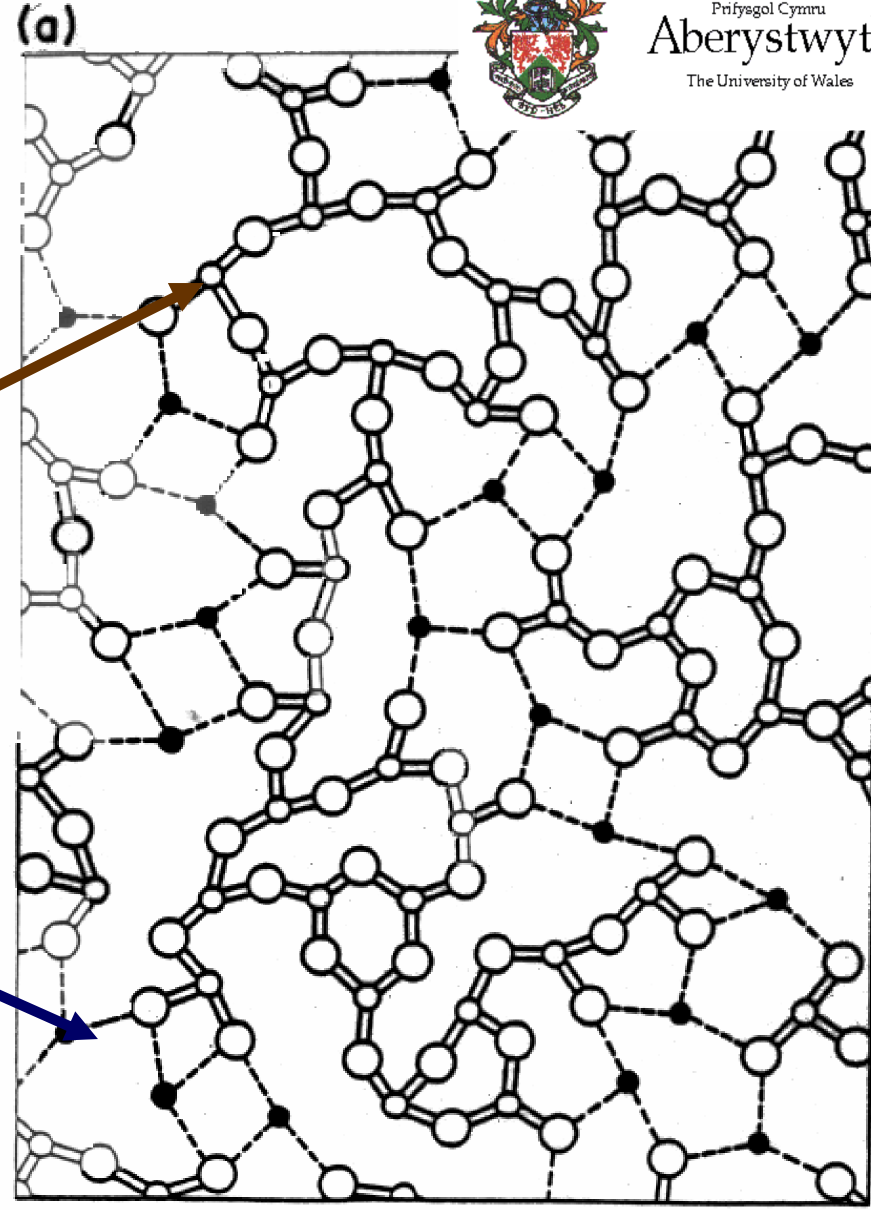
Modified Random Network

network

SiO_2 72.5%

modifiers

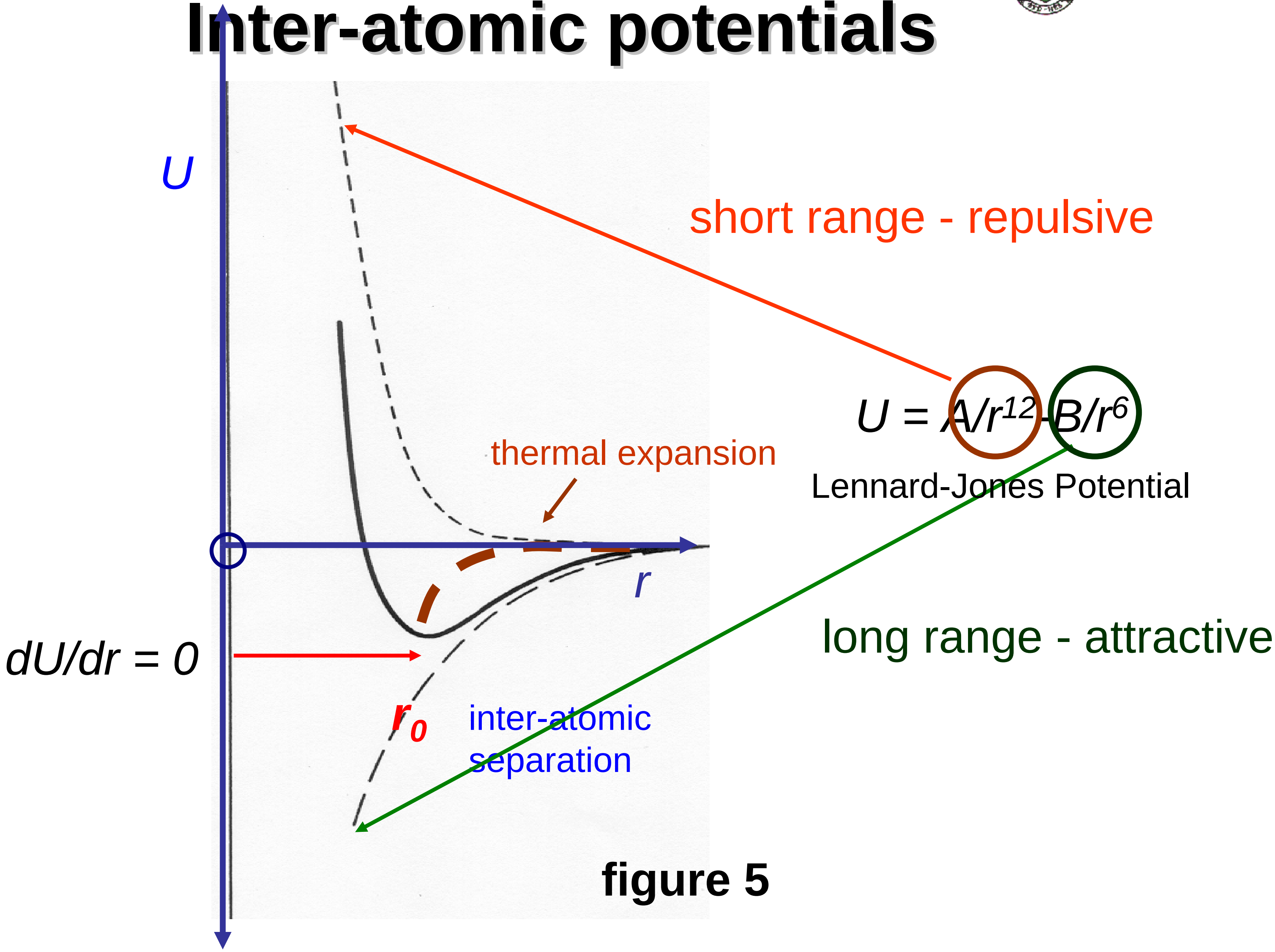
Na_2O 28.5%



EXAFS and The Structure of Glass

Greaves G N, J. Non-Cryst. Solids, 71, 203-217 (1985)

Inter-atomic potentials

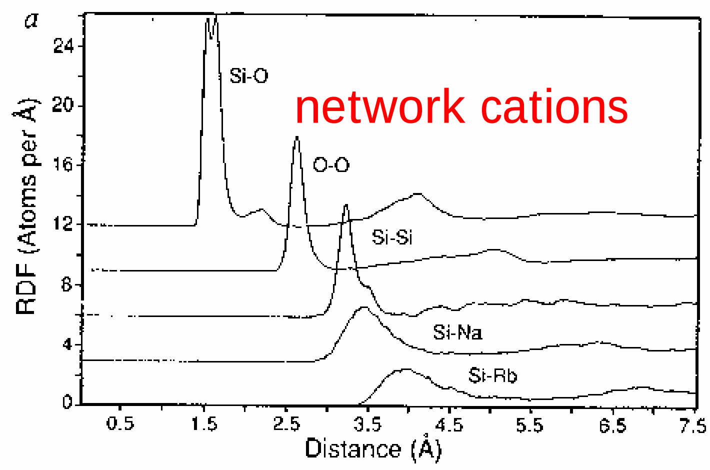


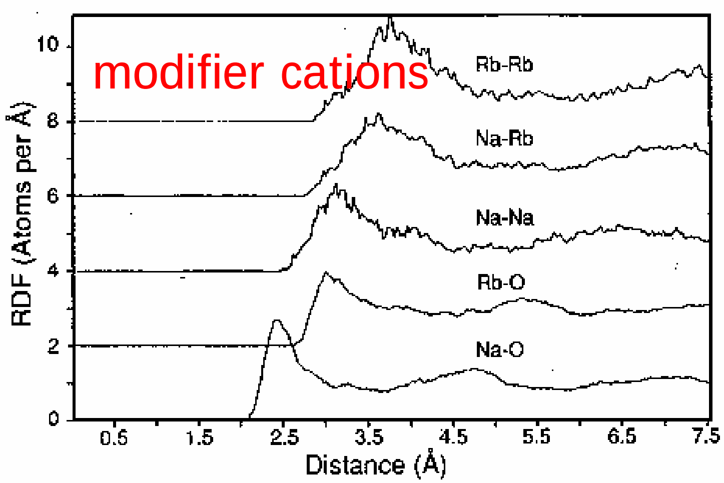
$U = A/r^{12} - B/r^{6}$

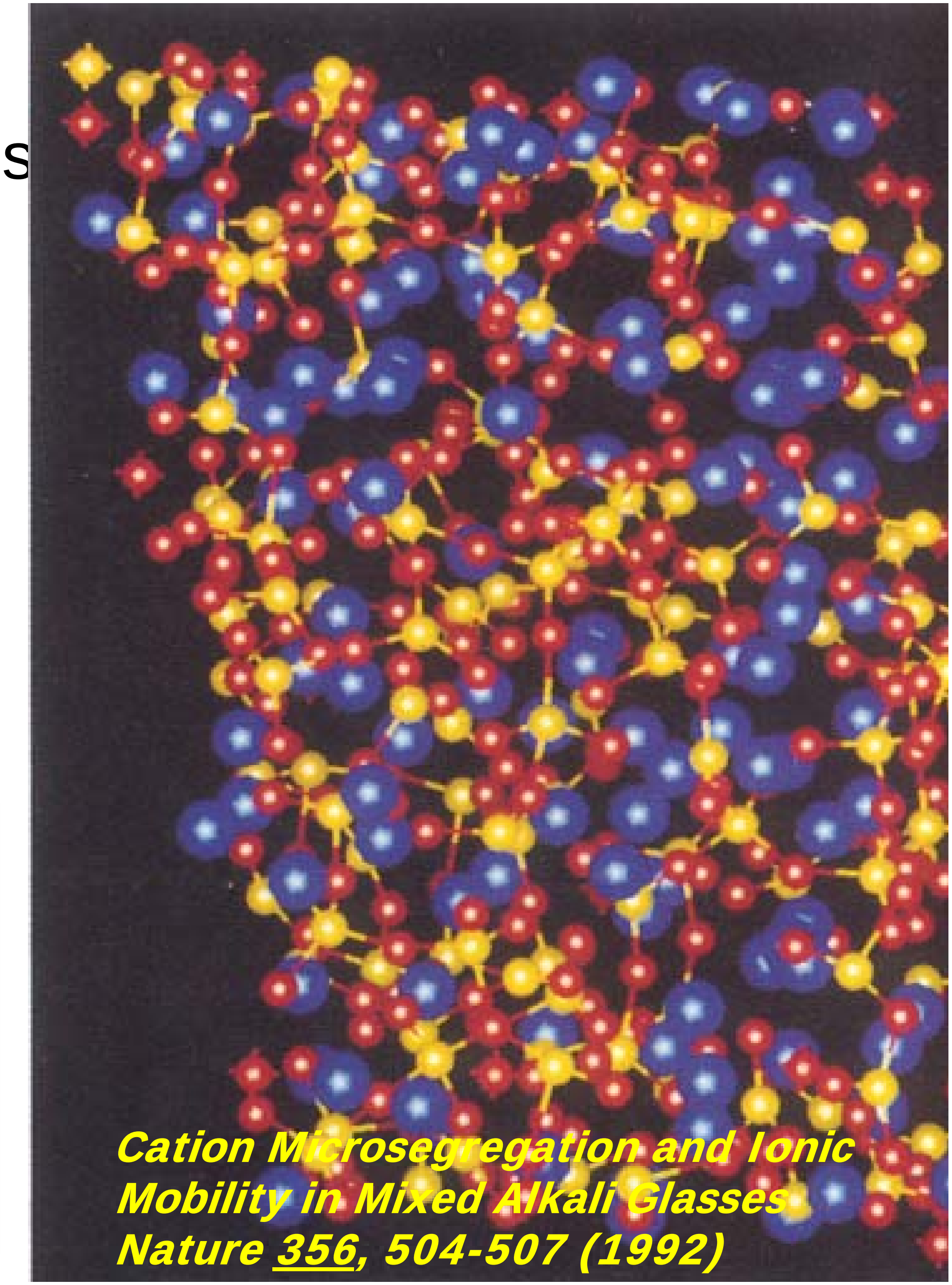
Lennard-Jones Potential

MD Simulation

Pair Distribution Functions and Alkali Channels







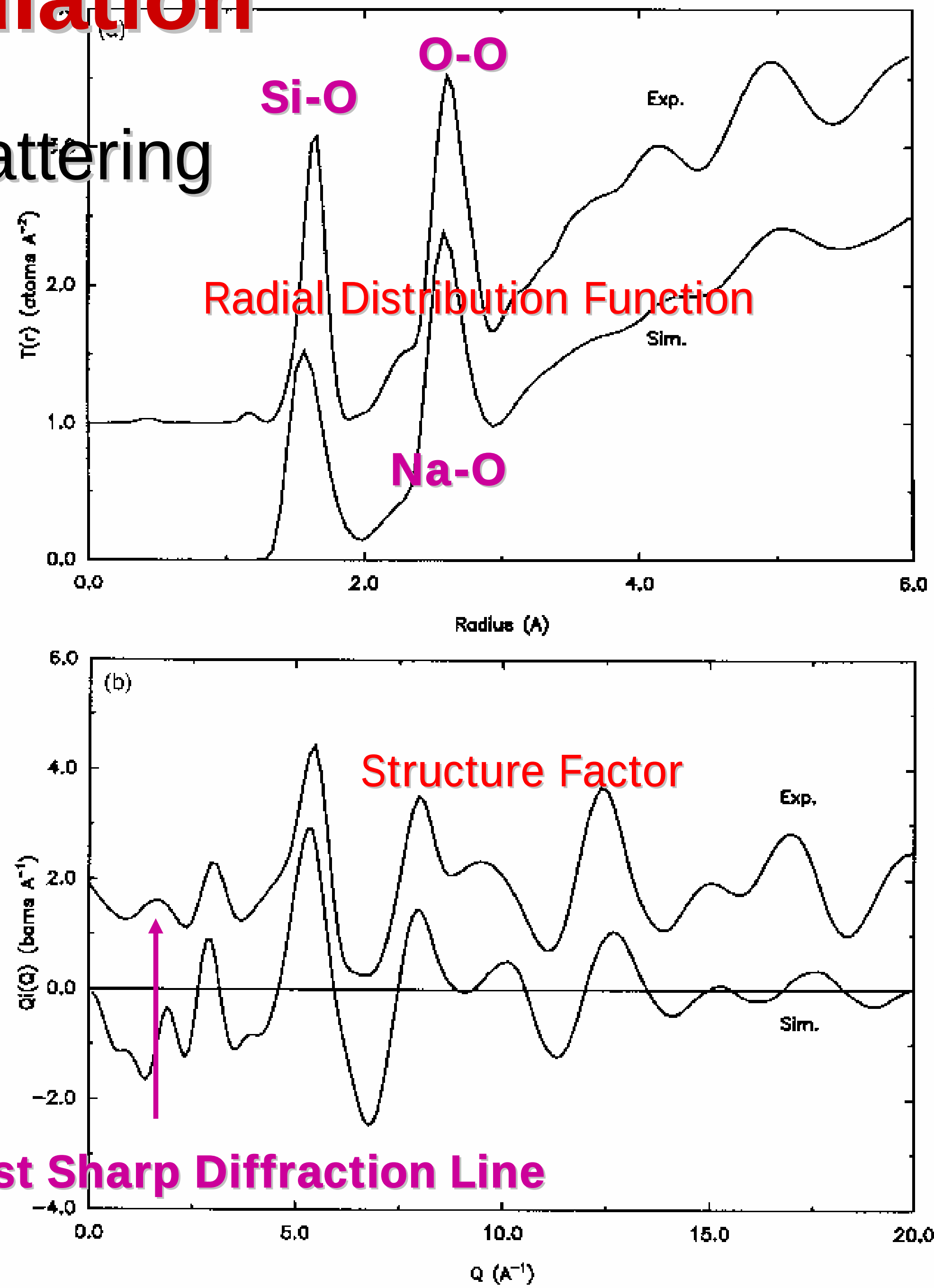
Cation Microsegregation and Ionic Mobility in Mixed Alkali Glasses
Nature <u>356</u>, 504-507 (1992)

MD Simulation

compared to

Neutron Scattering

$Na_2Si_2O_5$ Glass



Computer Simulation of Sodium Disilicate Glass

Smith W, Greaves GN and Gillan MJ

J. Chem. Phys. 103, 3091-3097 (1995)

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MD Simulation- Modelling Ionic Diffusion

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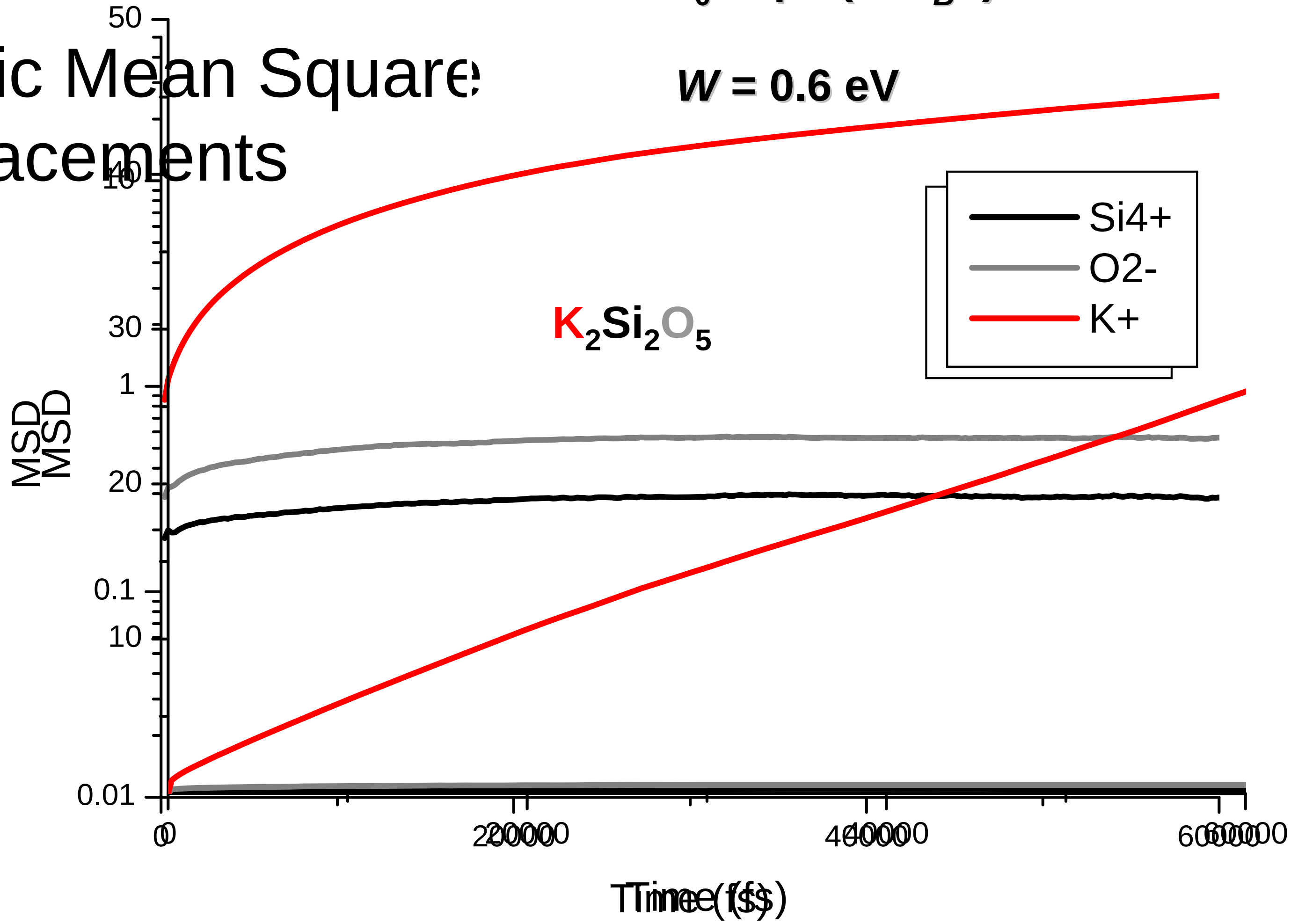
$D=1/6\ d(MSD)dt$

$$D = D_0 \exp -(W/k_B T)$$

$$W = 0.6\ \text{eV}$$

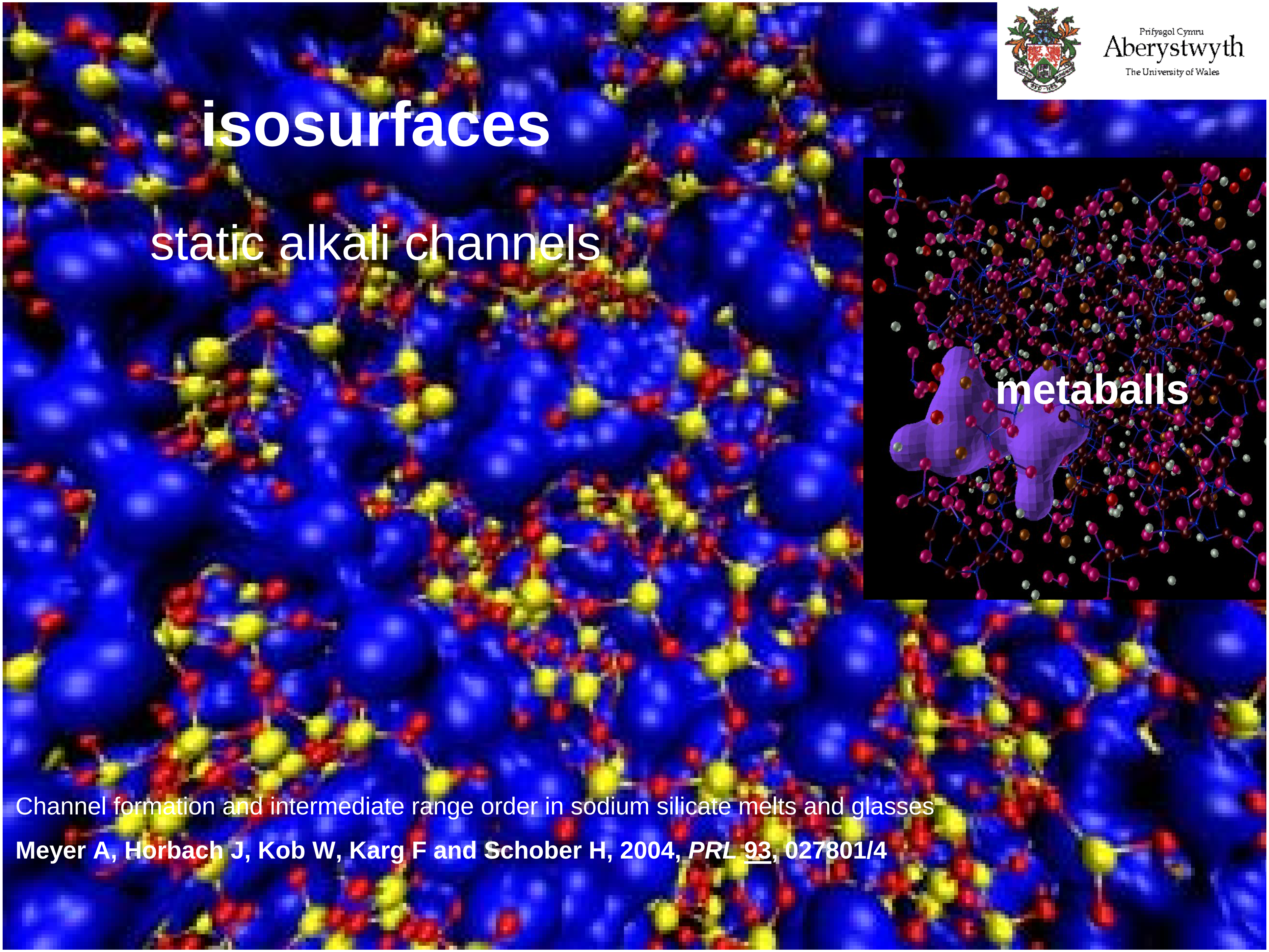
Atomic Mean Square Displacements



Virtual Reality Techniques – isosurfaces, ion tracks

isosurfaces

static alkali channels



Channel formation and intermediate range order in sodium silicate melts and glasses

Meyer A, Horbach J, Kob W, Karg F and Schober H, 2004, *PRL* 93, 027801/4

network isosurface

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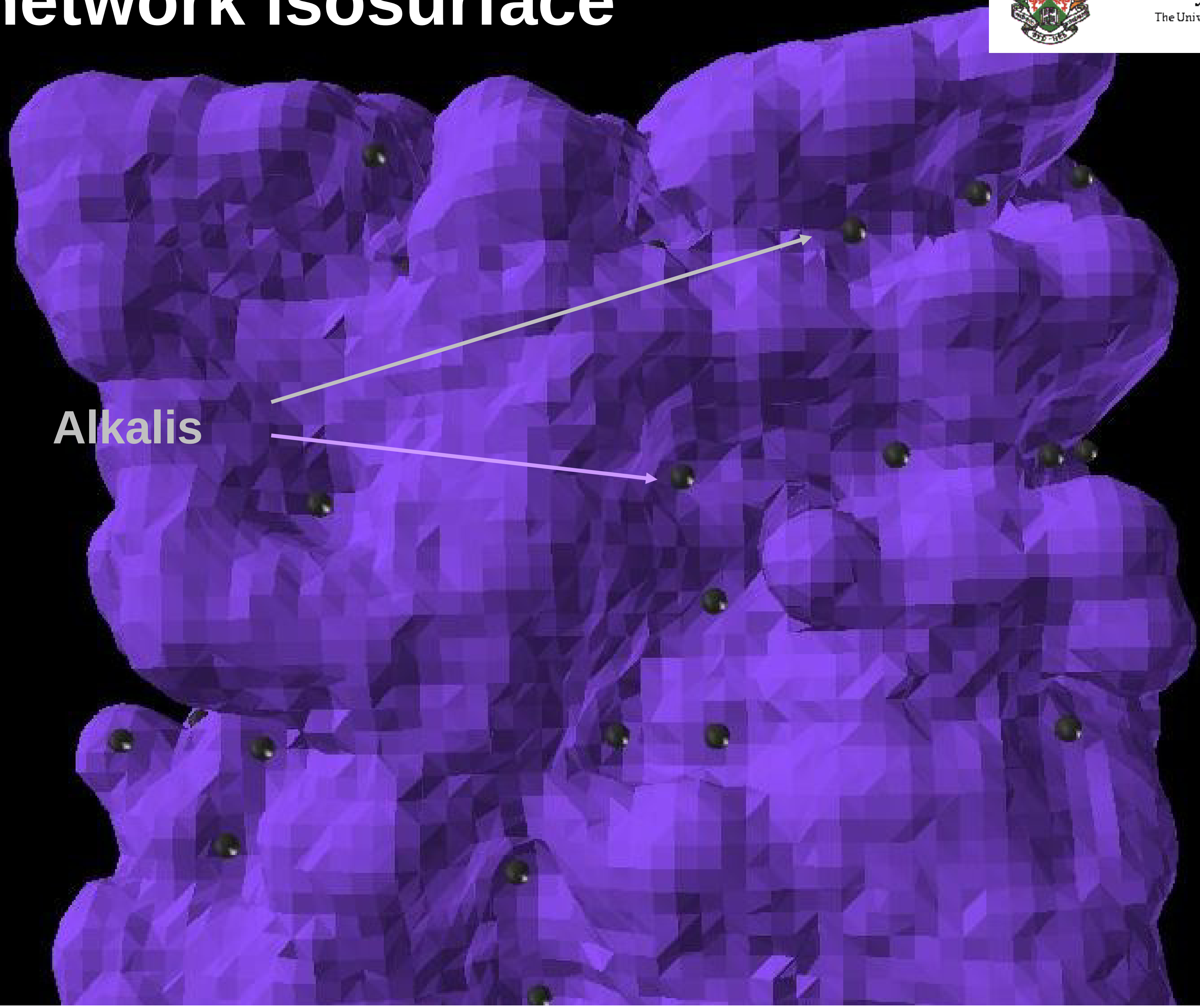
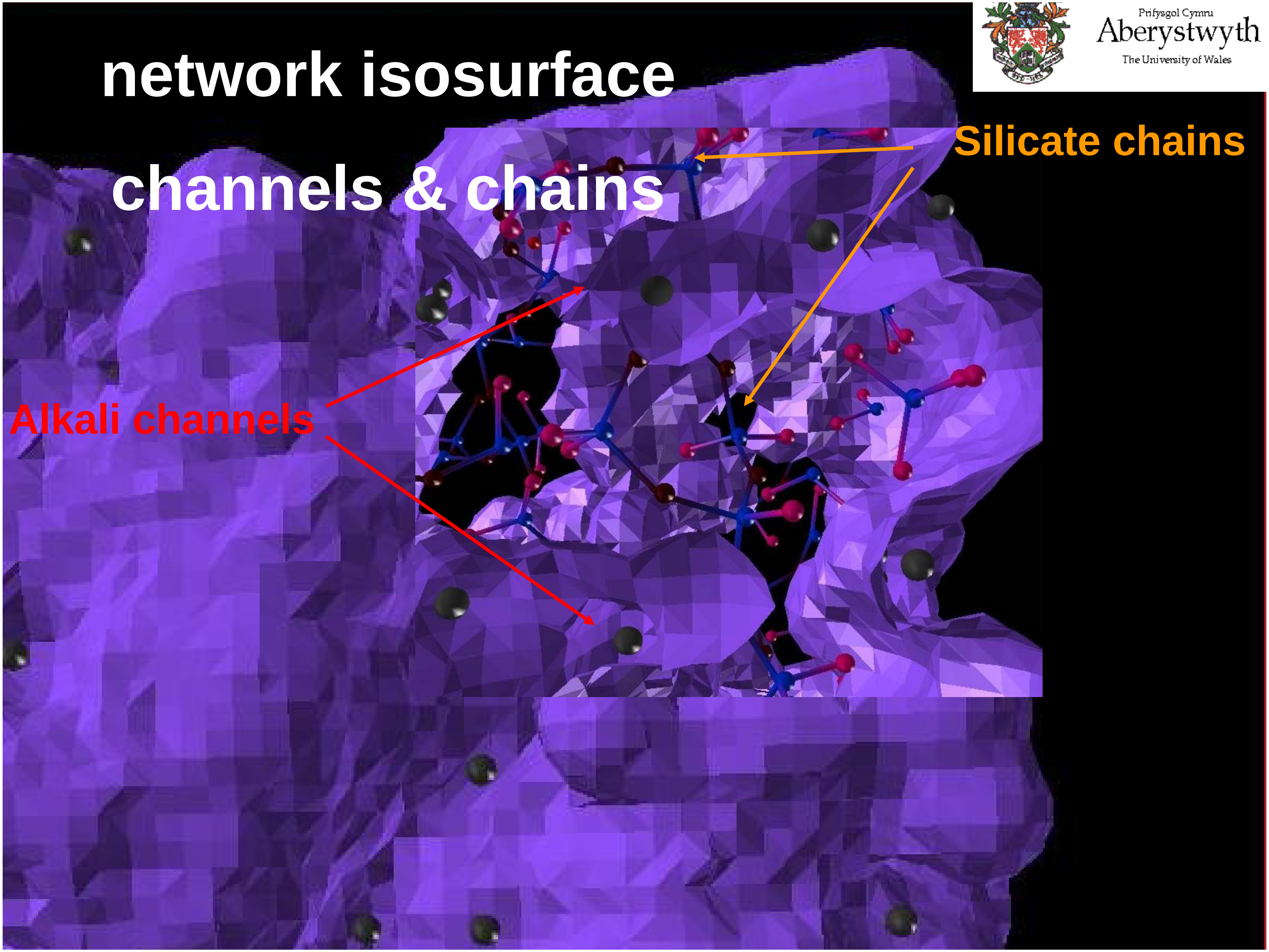


network isosurface

channels & chains




network isosurface
channels & chains
K
K
K
K
K
K
K
O
O
O
O
Si
$K_2Si_2O_5$ 1800K 5fs per frame

Ion tracks - $K_2Si_2O_5$

correlated alkali motion

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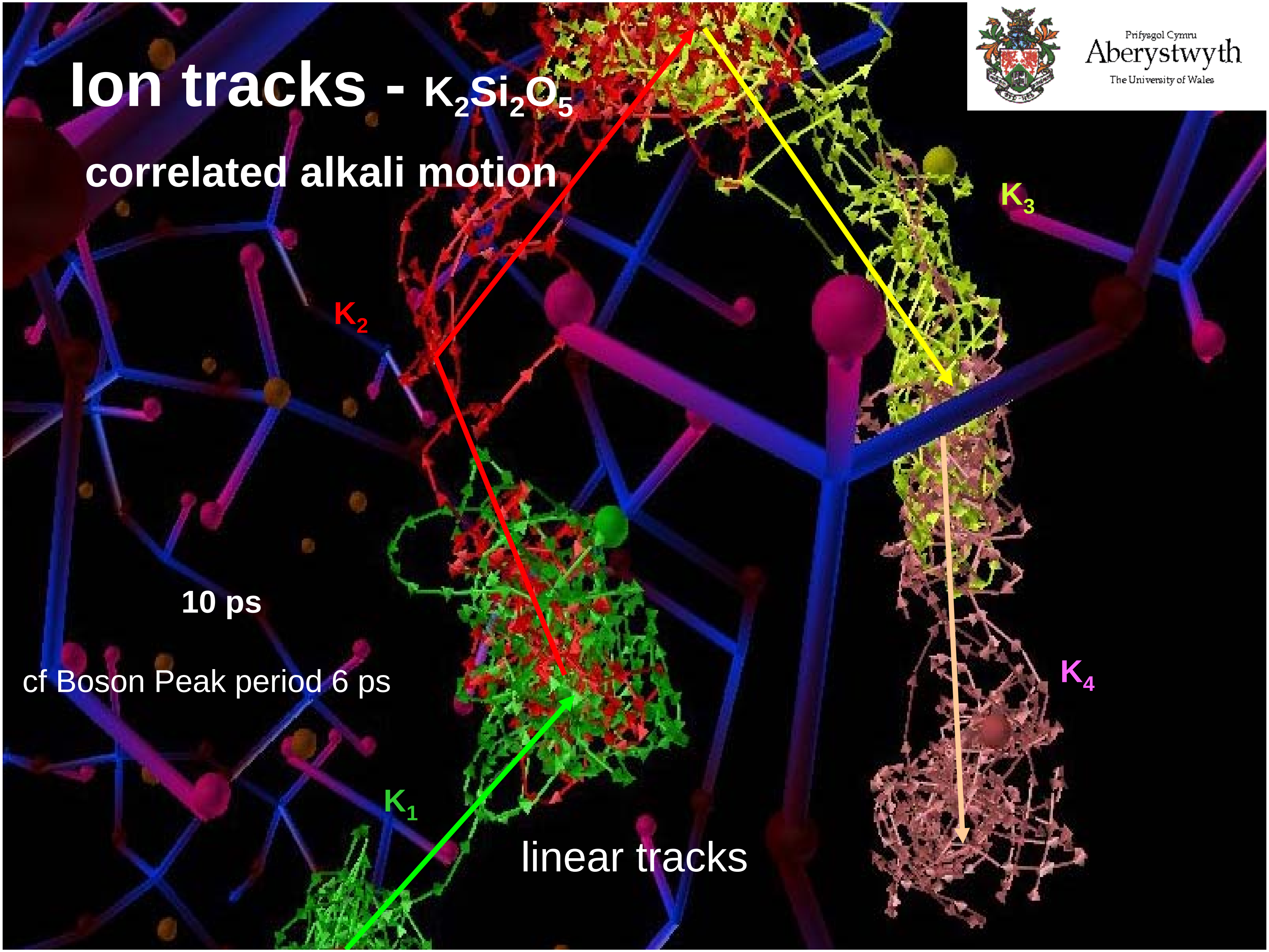
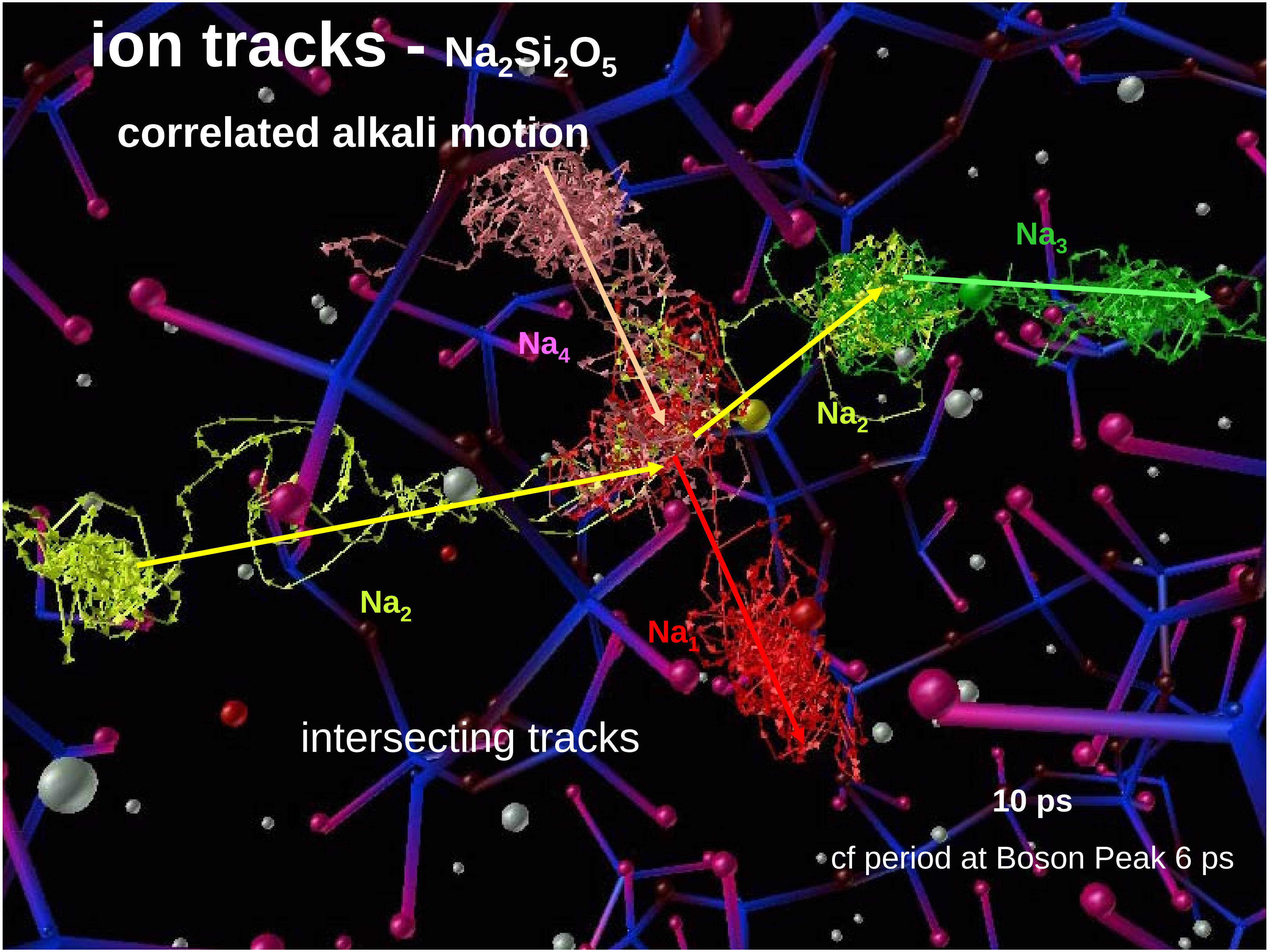
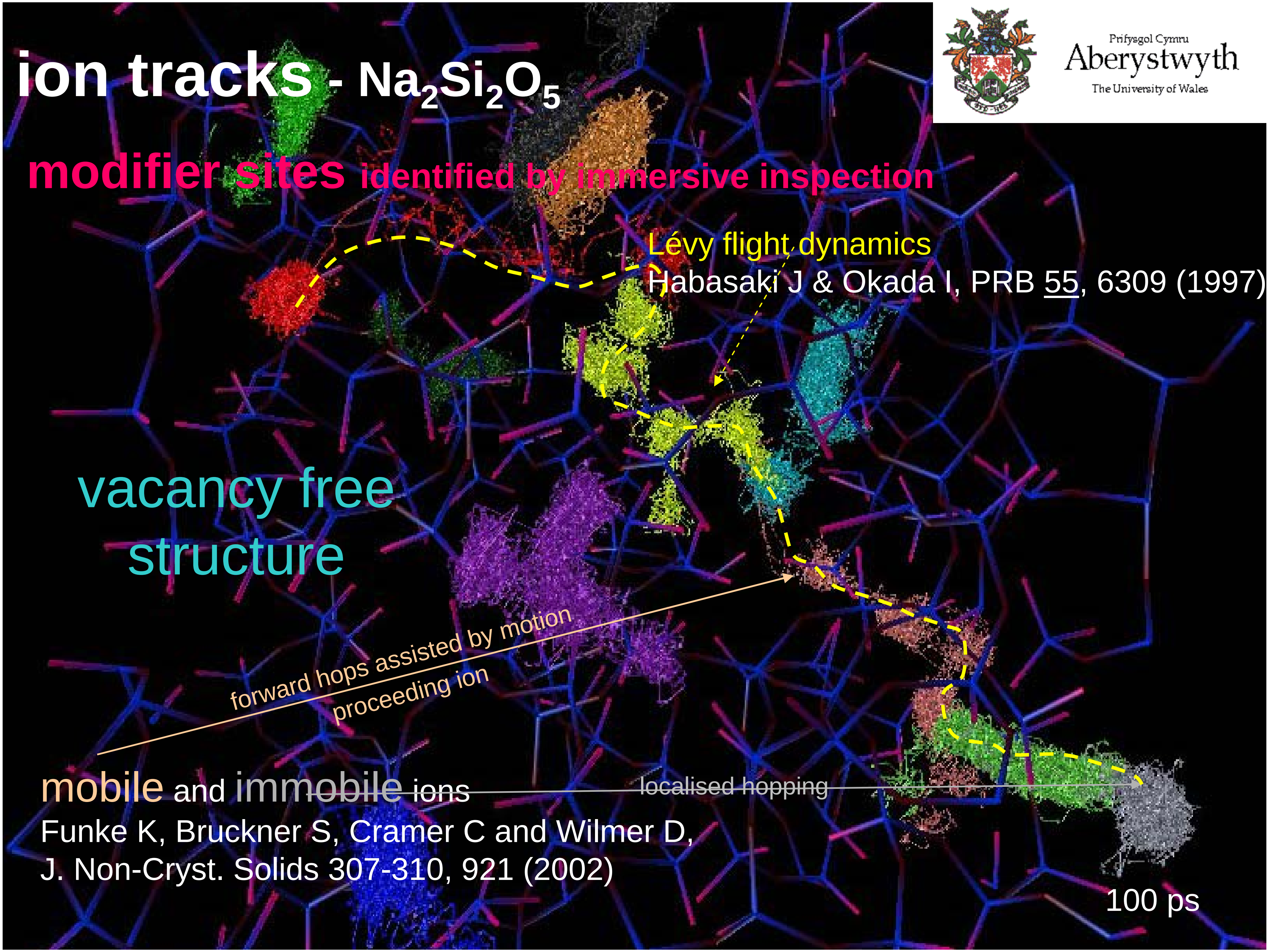



ion tracks - $Na_2Si_2O_5$
correlated alkali motion
Na_4
Na_3
Na_2
Na_2
Na_1
intersecting tracks
10 ps
cf period at Boson Peak 6 ps

Visualising cooperative dynamics – local frequencies


ion tracks - $Na_2Si_2O_5$
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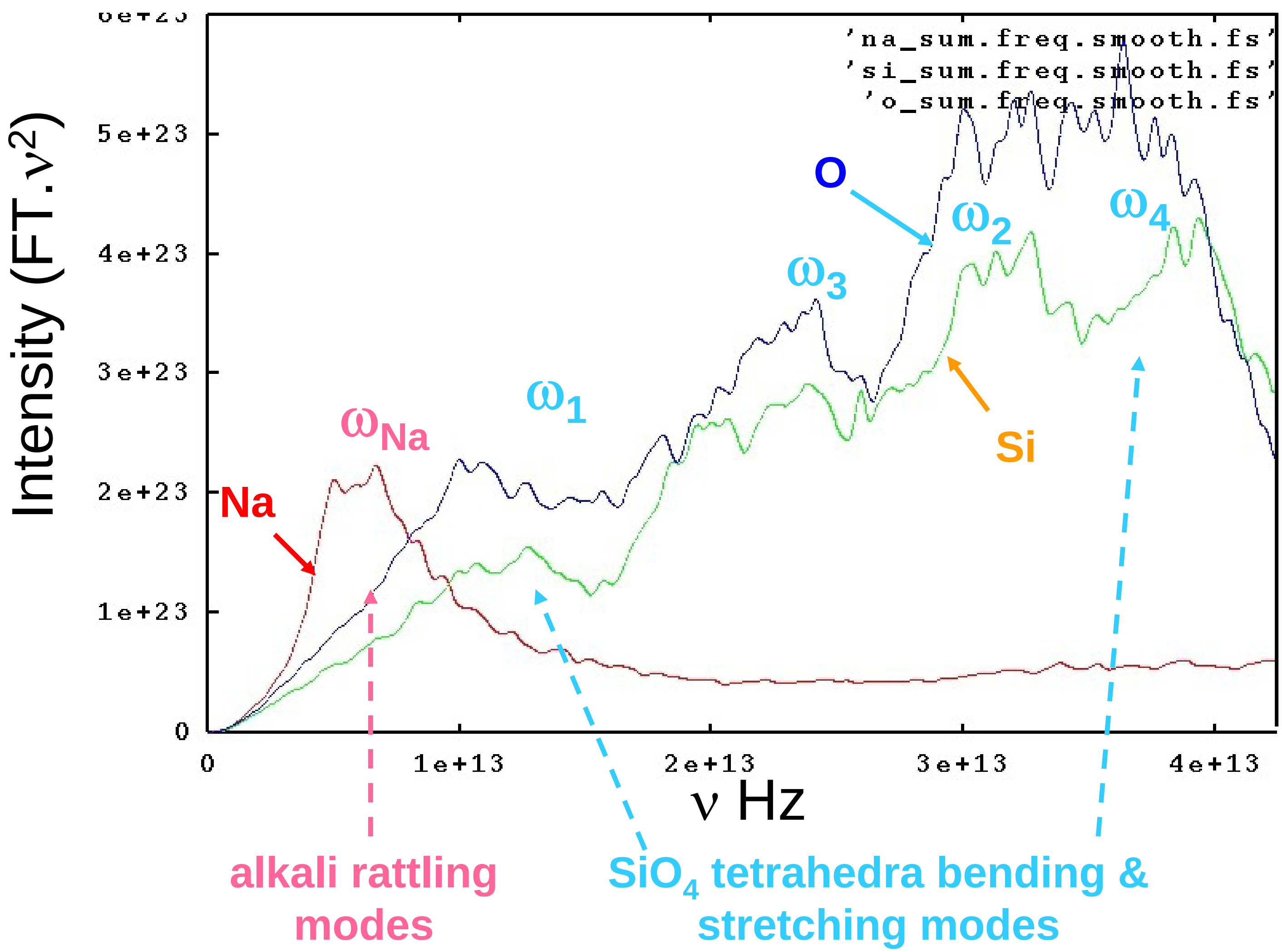
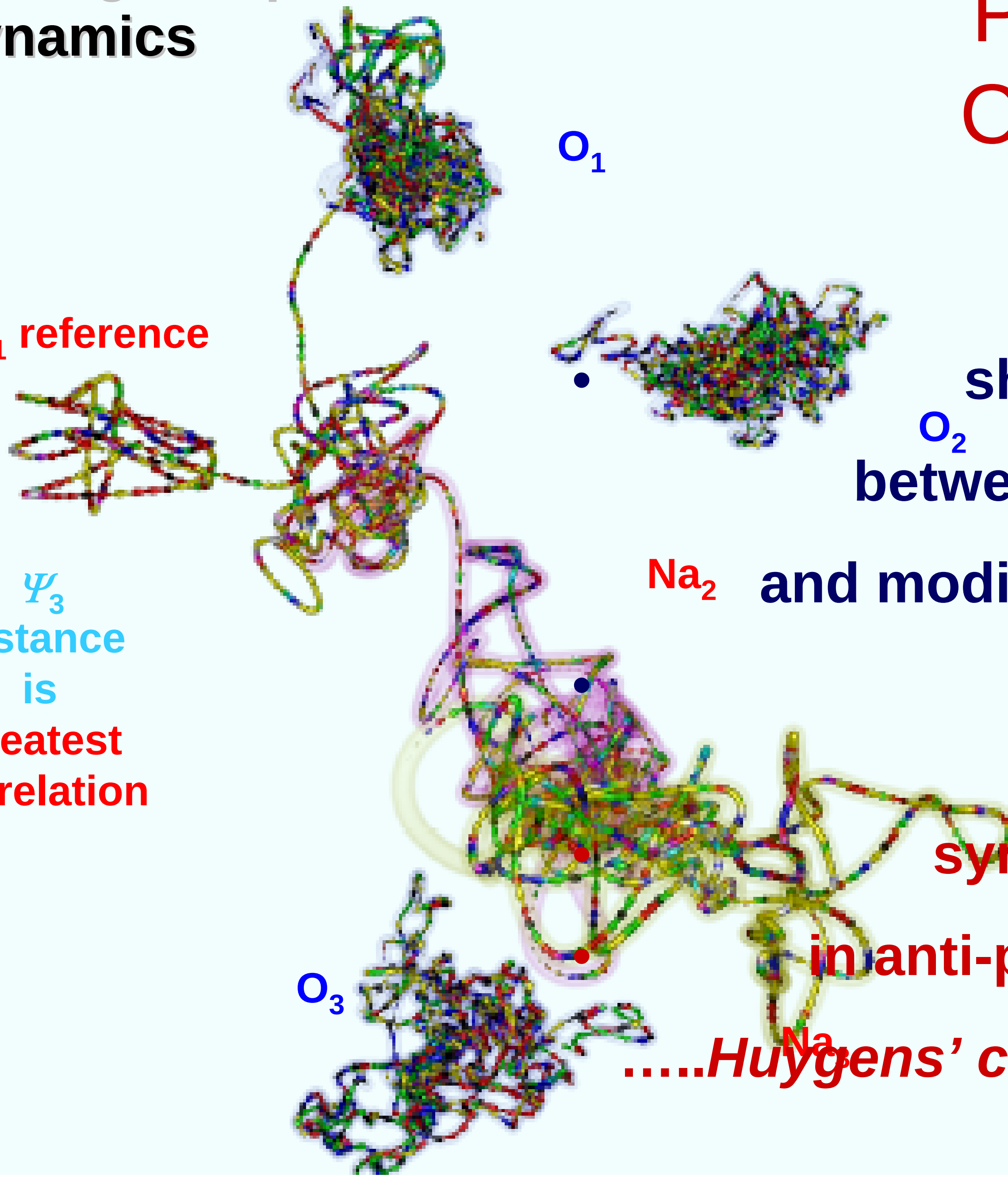
modifier sites identified by immersive inspection
Lévy flight dynamics
Habasaki J & Okada I, PRB 55, 6309 (1997)
vacancy free structure
forward hops assisted by motion
proceeding ion
mobile and immobile ions
localised hopping
Funke K, Bruckner S, Cramer C and Wilmer D,
J. Non-Cryst. Solids 307-310, 921 (2002)
100 ps

local frequencies – sodium, oxygen, silicon



Positional Correlation

visualising co-operative ion dynamics



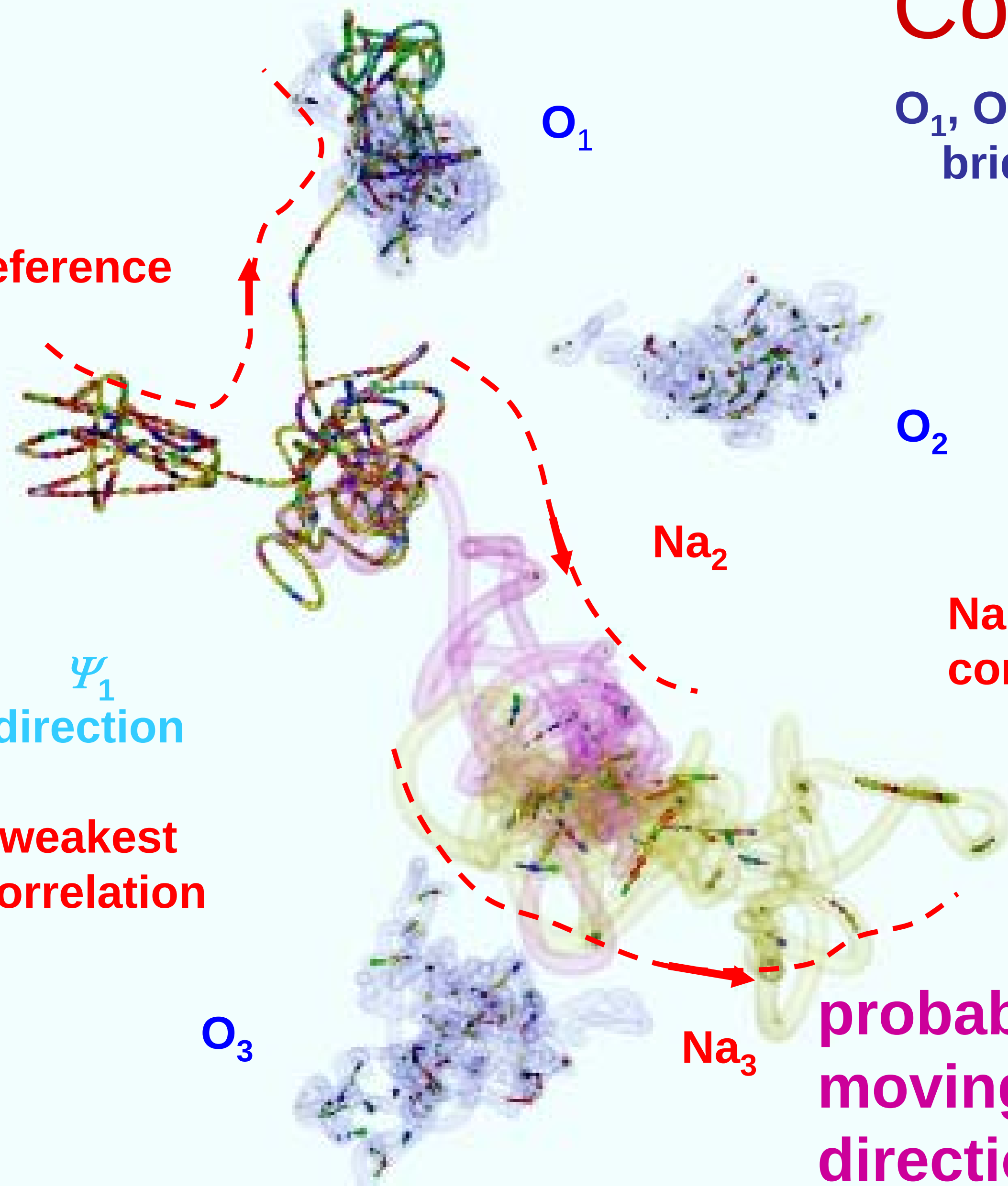
shared frequencies
between network (NBO)
and modifiers (Na)

alkalis
approximately
synchronised
in anti-phase

…..Huygens' clocks….

visualising cooperative ion dynamics

Directional Correlation

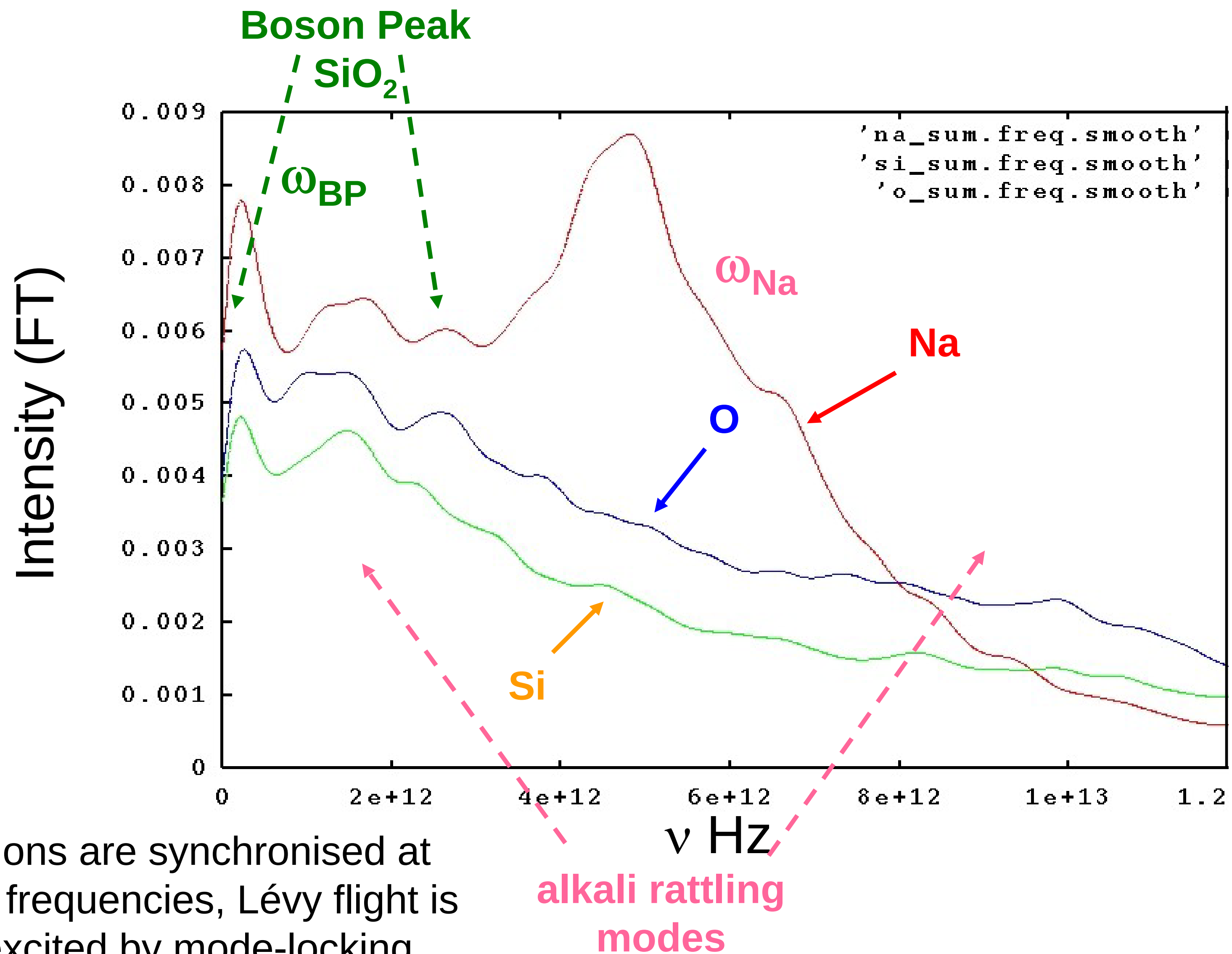


O_1, O_2 and O_3 are shared non-bridging oxygens (NBOs)

Na_1, Na_2 and Na_3 involved in correlated motion over 10ps

probability is that ions are moving in opposite directions

shared low frequencies – sodium, oxygen, silicon



if ions are synchronised at low frequencies, Lévy flight is excited by mode-locking behaviour

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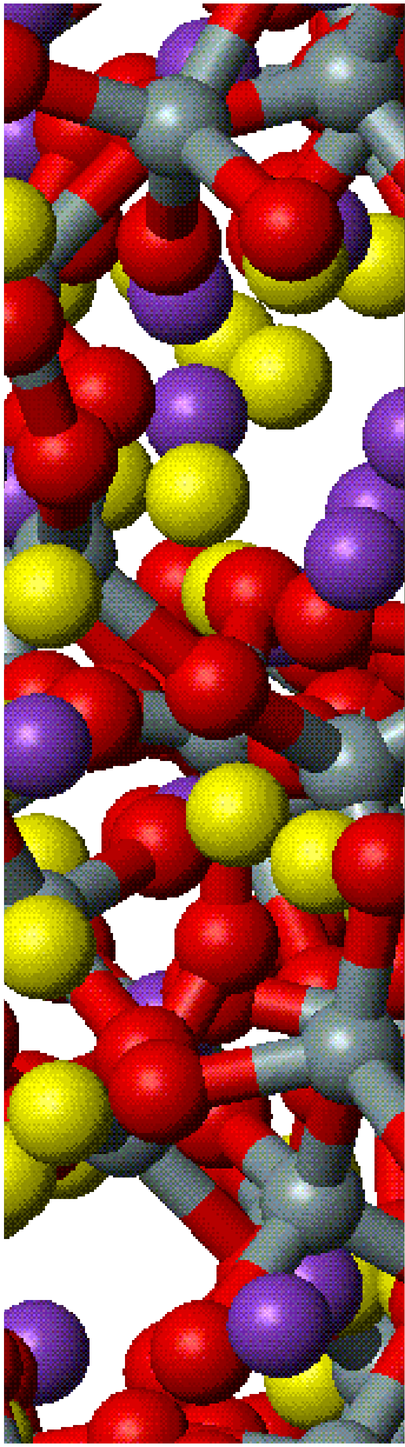

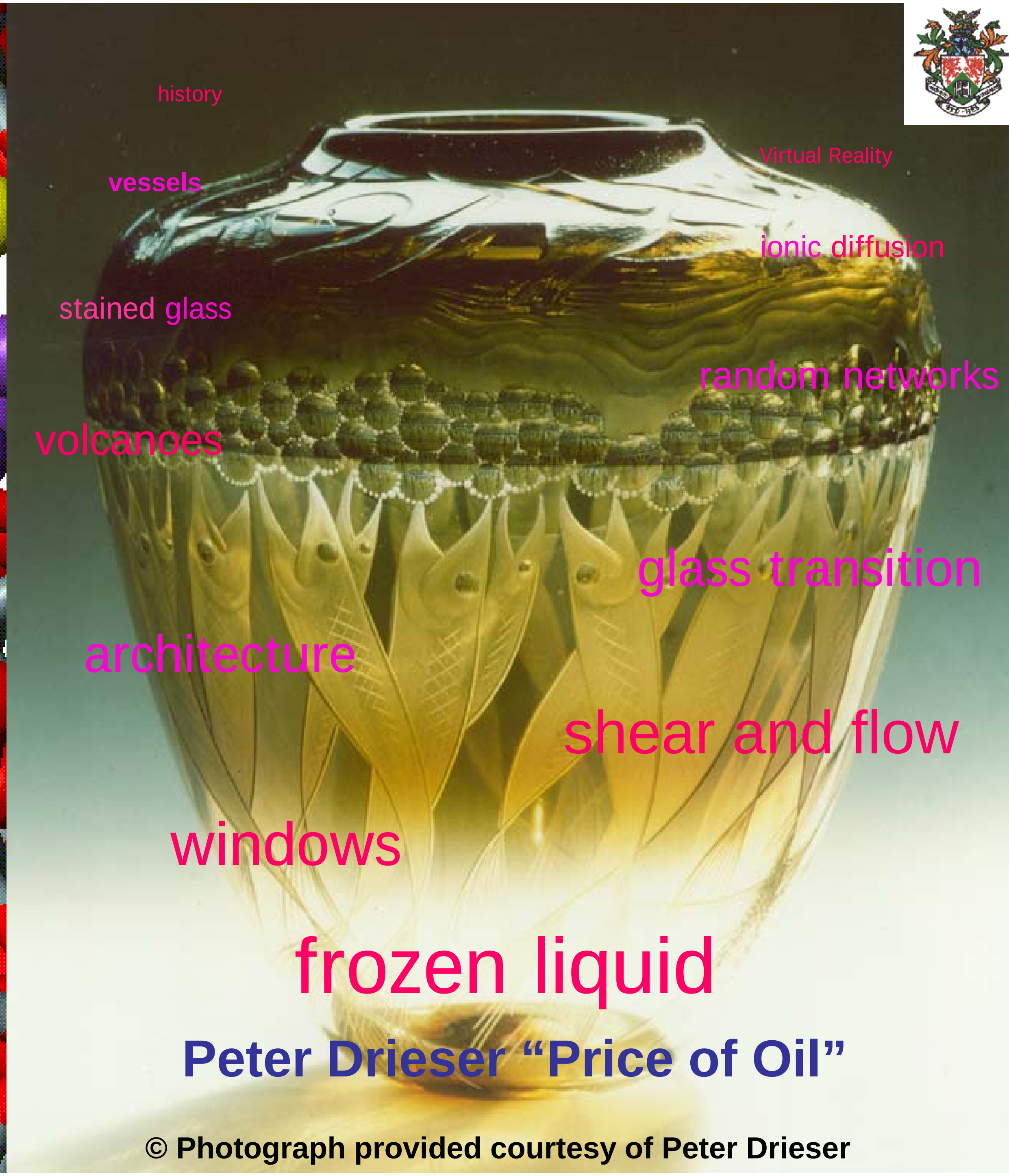

Peter Drieser "Price of Oil"

© Photograph provided courtesy of Peter Drieser