

Materiali Amorfi

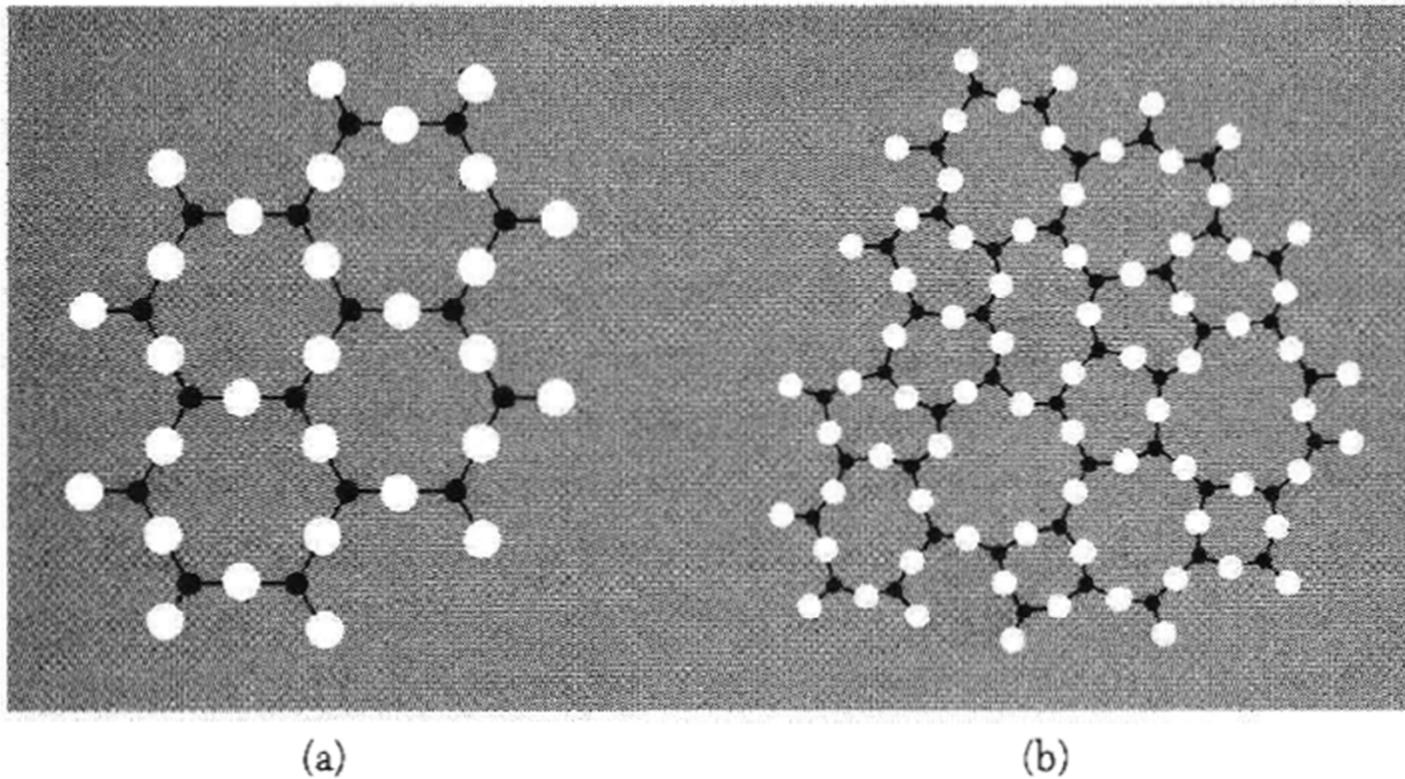


Figure 4 Schematic two-dimensional analogs illustrating the differences between: (a) the regularly repeating structure of a crystal and (b) continuous random network of a glass. (After Zachariasen.)

Amorfo vs Vetro

GLASSES

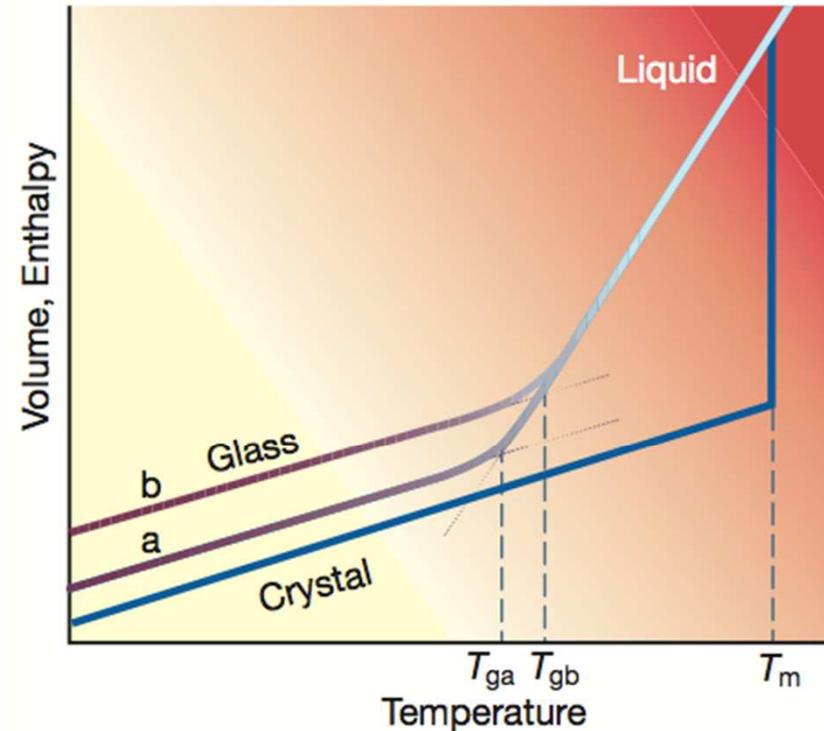
A glass has the random structure of the liquid from which it is derived by cooling below the freezing point, without crystallization. Also, a glass has the elastic properties of an isotropic solid.

By general agreement, we say that a liquid on being cooled becomes a glass when the viscosity equals 10^{13} poise, where a poise is the CGS unit of viscosity.¹ This defines the **glass transition temperature** T_g . At temperatures above T_g we have a liquid; below T_g we have a glass. The transition is not a thermodynamic phase transition, only a transition for “practical purposes.”

¹The SI unit of viscosity is 1 Nsm^{-2} , so that $1 \text{ poise} = 0.1 \text{ Nsm}^{-2}$. It is quite common to find viscosities given in cp or centipoise, being 10^{-2} poise.

Amorfo vs vetro

Figure 1 Temperature dependence of a liquid's volume v or enthalpy h at constant pressure. T_m is the melting temperature. A slow cooling rate produces a glass transition at T_{ga} ; a faster cooling rate leads to a glass transition at T_{gb} . The thermal expansion coefficient $\alpha_p = (\partial \ln v / \partial T)_p$ and the isobaric heat capacity $c_p = (\partial h / \partial T)_p$ change abruptly but continuously at T_g .



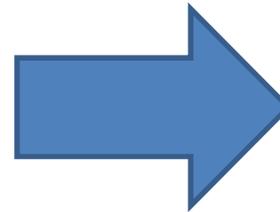
Modelli strutturali

Continuous Random Network (CRN)

Microcristalliti

Metodo Monte Carlo

Molecular Dynamics



Confronto con figure
di diffrazione

Modelli strutturali

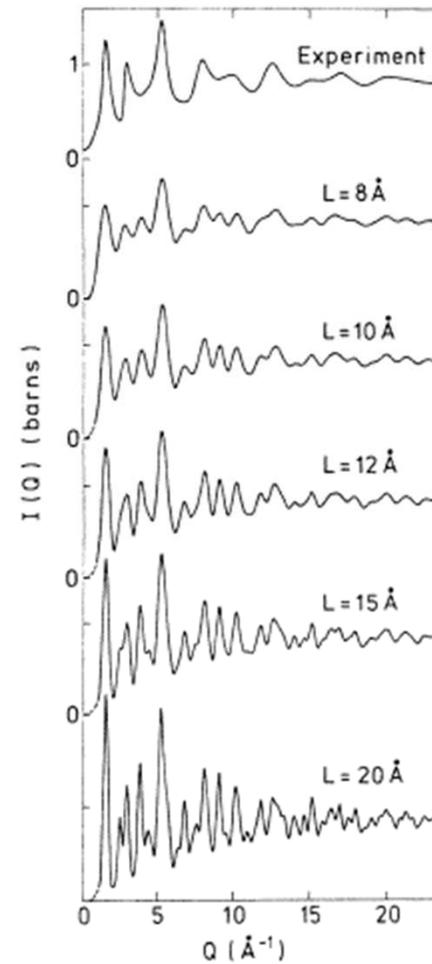


Figure 10. The corrected neutron diffraction pattern for vitreous SiO_2 compared to the results of quasi-crystalline model calculations, based on the β -cristobalite structure, as a function of the correlation length, L [40].

Modelli strutturali

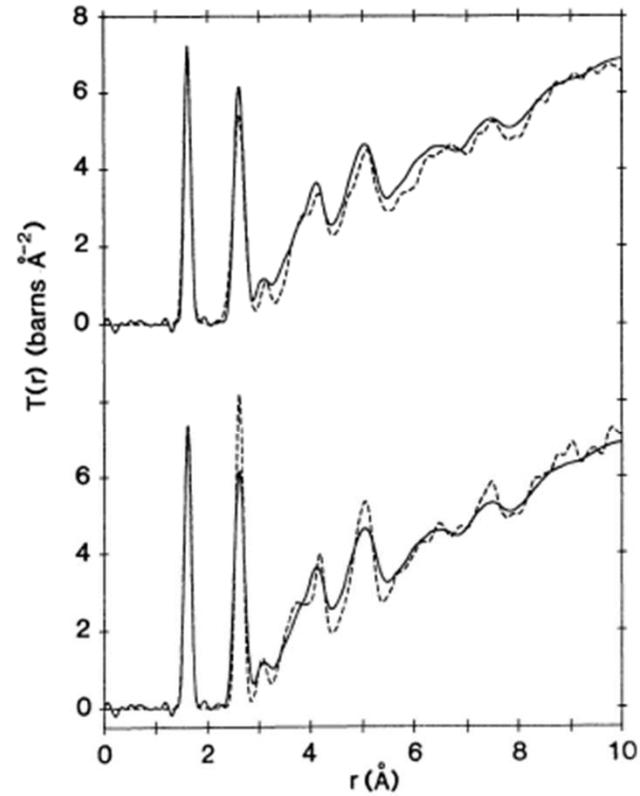


Figure 11. The neutron (upper curves) and X-ray (lower curves) correlation functions for the Bell and Dean [43] model of vitreous SiO_2 , as relaxed by Gaskell and Tarrant [44], (dashed line) compared to experiment (solid line).

Modelli strutturali

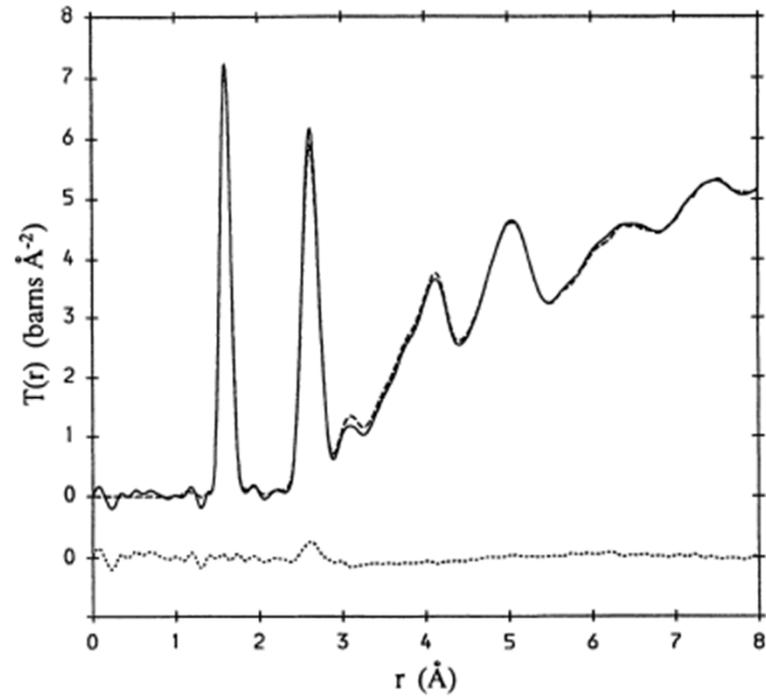


Figure 12. The neutron correlation function for a random network model of Gladden [45], refined using the reverse Monte Carlo technique, compared to experiment. —, experiment; ---, model and , residual.

Modelli strutturali

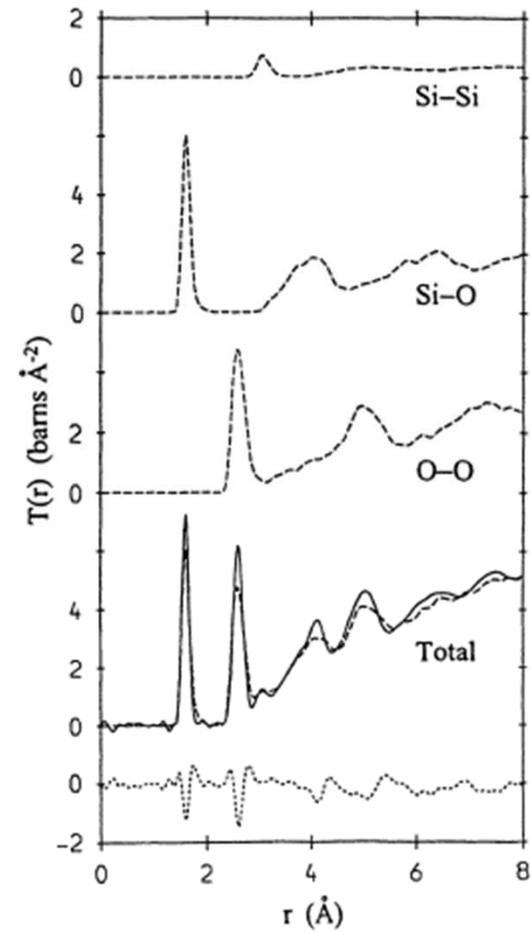


Figure 13. The neutron correlation function for the molecular dynamics simulation of vitreous SiO_2 by Vessal *et al.* [47], compared to the neutron data of Ref. [17] ($Q_{\text{max}} = 45.2 \text{ \AA}^{-1}$). —, experiment; ---, simulation and , difference curve (simulation - experiment).



a tetravalent metalloid, more reactive than germanium, the metalloid directly below it in the table. Controversy about silicon's character dates to its discovery. It was first prepared and characterized in pure form in 1823. In 1808, it was given the name silicium (from *Latin*: *silix*, hard stone or flint), with an **-ium** word-ending to suggest a *metal*, a name which the element retains in several languages. The present *English* name was first suggested in 1817 to conform with the physically similar elements, *carbon* and *boron*.

Silicon is the eighth most *common element* in the universe by mass, but very rarely occurs as the pure free element in the Earth's crust. It is most widely distributed in *dusts*, *sands*, *planetoids*, and *planets* as various forms of *silicon dioxide* (silica) or *silicates*. Over 90% of the Earth's crust is composed of *silicate minerals*, making silicon the *second most abundant element* in the Earth's crust (about 28% by mass) after *oxygen*.^[9]

Most silicon is used commercially without being separated, and often with little processing of the natural minerals. Such use includes industrial construction with *clays*, *silica sand*, and *stone*. Silicate is used in *Portland cement* for *mortar* and *stucco*, and mixed with silica sand and *gravel* to make *concrete* for walkways, foundations, and roads. Silicates are used in whiteware *ceramics* such as *porcelain*, and in traditional *quartz-based soda-lime glass* and many other specialty *glasses*. Silicon

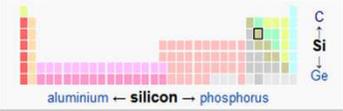


Spectral lines of silicon

General properties

Name, symbol	silicon, Si
Appearance	crystalline, reflective with bluish-tinged faces
Pronunciation	<i>/ˈsɪlɪkən/</i> or <i>/ˈsɪlɪkɒn/</i> <i>SIL-ə-ken</i> or <i>SIL-ə-kon</i>

Silicon in the periodic table



aluminium ← **silicon** → phosphorus

Atomic number (Z) 14

Group, block group 14 (carbon group), p-block

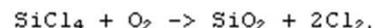
Il biossido di silicio amorfo: $\alpha\text{-SiO}_2$, o silice

Silice

Da Wikipedia, l'enciclopedia libera.

La **silice** /silice/ (o anche **anidride silicica**, IUPAC **biossido di silicio**) è un composto del silicio la cui formula chimica è SiO_2 .

La silice purissima per applicazioni ad alta tecnologia viene ottenuta dalla reazione in fiamma fra il **tetracloruro di silicio** e l'**ossigeno**



e a seconda del contenuto finale di gruppi OH, la silice viene comunemente distinta in silice dry e silice wet (rispettivamente, basso o elevato contenuto di gruppi OH).

Pura, è una polvere cristallina bianca che impartisce all'acqua una lieve **acidità**: una **sospensione** di 40 g in un litro di acqua ha **pH** compreso tra 3,7 e 4,7.

Lo stato fisico più comune in natura è quello solido cristallino, in **minerali** come il **quarzo** e i suoi **polimorfi**, e più raramente quello amorfo, come nell'**opale**; la silice cristallina è il costituente principale di diverse **rocce sedimentarie** (ad es. **sabbia**, **radiolariti**, **quarzareniti** e **pelle di leopardo**). Talvolta si rinviene cristallizzata da fluidi di segregazione all'interno di **rocce metamorfiche** e **magmatiche** e all'interno di **rocce carbonatiche** sotto forma di **selce** di origine **metasomatica**.

Moltissimi animali e piante utilizzano la silice presente come ione silicato sia nell'acqua dolce sia in quella salata purché al di sotto dei 18 °C. Le **diatomee**, i **radiolari**, le **spugne silicee**, moltissimi **cereali** ed altre piante come la **canna da zucchero** e l'**equiseto** utilizzano questo materiale come impalcatura per lo sviluppo di strutture scheletriche.

Esistono comunque anche 15 **solidi cristallini** composti esclusivamente di silice, tra i quali il più famoso è certamente il **quarzo** o le sue forme di alta e altissima temperatura **tridimite** e **cristobalite**, oltre a solidi criptocristallini quali il **calcedonio**.

Silice	
	
Nome IUPAC	
diossido di silicio	
Caratteristiche generali	
Formula bruta o molecolare	SiO_2
Peso formula (u)	60,08
Aspetto	solido cristallino bianco
Numero CAS	[7631-86-9]
Proprietà chimico-fisiche	
Densità (g/cm^3 , in c.s.)	2,2
Solubilità in acqua	0,15 g/l a 298 K
Temperatura di fusione (K)	1999 (1726 °C)
Proprietà termochimiche	
$\Delta_f H^\circ$ ($\text{kJ}\cdot\text{mol}^{-1}$)	-910,7
$\Delta_f G^\circ$ ($\text{kJ}\cdot\text{mol}^{-1}$)	-856,3
S_m° ($\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$)	41,5
$C_{p,m}^\circ$ ($\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$)	44,4

Il biossido di silicio amorfo: $\alpha\text{-SiO}_2$, o silice

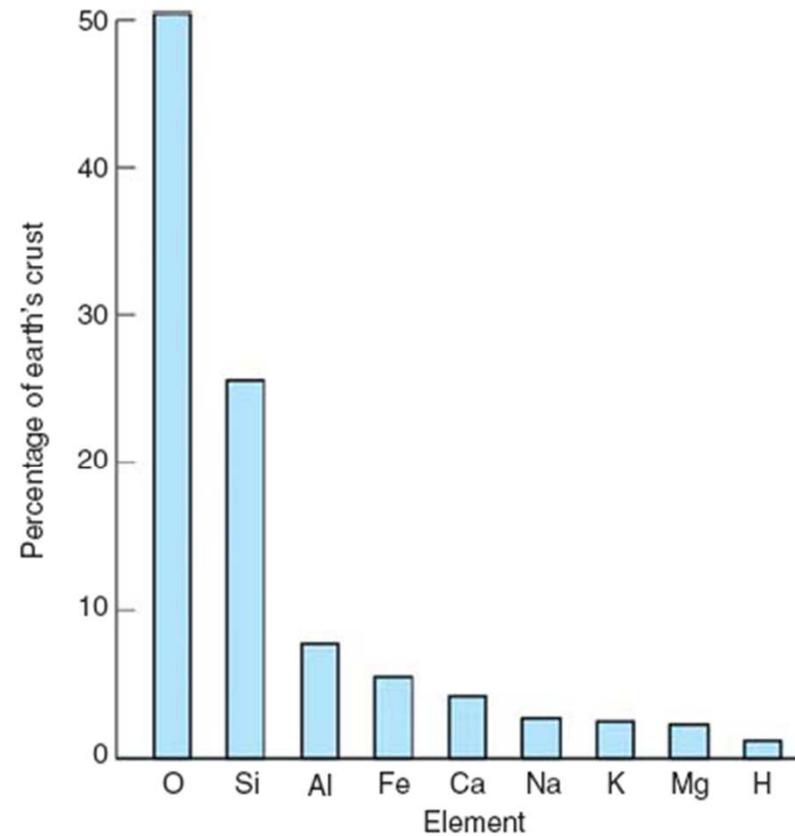


Fig. 1 The relative abundance of elements in the earth's crust illustrates the common availability of quartz and the silicas [1]

Il biossido di silicio amorfo: $\alpha\text{-SiO}_2$, o silice

• Batteriologicamente pura alla sorgente • Oligominerale NAT

ANALISI CHIMICA E CHIMICO FISICA
UNIVERSITÀ DEGLI STUDI DI CATANIA
DIPARTIMENTO DI IGIENE E SANITÀ
DETERMINAZIONI CHIMICO-FISICHE
EVALUTAZIONI CHIMICHE DIVERSE

UNIVERSITY STUDY CATANIA
CHEMICAL ANALYSIS

Temperatura dell'acqua	11,6°C	Water temp. at spring	11,6°C
Cond. Elett. Spec. A 20°C (k20)	100uS/cm ⁻¹	Conductivity 20°C	100uS/cm ⁻¹
(Ph)	6,6	(Ph)	6,6
Residuo fisso a 180°	70 mg/l	Residue 180°	70 mg/l
Azoto ammoniacale	<0,03 mg/l	Ammonium	<0,03 mg/l
Nitriti (NO ₂)	<0,002 mg/l	Nitrites (NO ₂)	<0,002 mg/l
Nitrati (NO ₃)	2,70 mg/l	Nitrates (NO ₃)	2,70 mg/l

Gas disciolti in un litro d'acqua
Anidride carbonica libera (CO₂) 0,016 g/l
Ossidabilità (O₂) 1,40 mg/l

Dissolved gas per litre of water
Carbon dioxide at the source (LU₂) 0,016 g/l
Oxidability (O₂) 1,40 mg/l

Sostanze disciolte in un litro d'acqua

CALCIO	CA ⁺⁺	3,60 mg/l
SODIO	NA ⁺	0,013 g/l
MAGNESIO	Mg ⁺⁺	4,60 mg/l
POTASSIO	K ⁺	0,23 mg/l
BICARBONATI	HCO ₃	42,70 mg/l
SOLFATI	SO ₄	4,86 mg/l
CLORURI	CL	3,90 mg/l
SILICE	SiO ₂	26,43 mg/l

Mineral content per litre

CALCIUM	CA ⁺⁺	3,60 mg/l
SODIUM	NA ⁺	0,013 g/l
MAGNESIUM	Mg ⁺⁺	4,60 mg/l
POTASSIUM	K ⁺	0,23 mg/l
BICARBONATE	HCO ₃	42,70 mg/l
SULPHATE	SO ₄	4,86 mg/l
CHLORIDE	CL	3,90 mg/l
SICON	SiO ₂	26,43 mg/l

Classificazione Acqua Oligominerale
Catania, 05/11/2010
Il RESPONSABILE - Prof. S. Sciacca

Catania, 05/11/2010
MANAGER - Prof. S. Sciacca

Silice	
	
Nome IUPAC	
diossido di silicio	
Caratteristiche generali	
Formula bruta o molecolare	SiO ₂
Peso formula (u)	60,08
Aspetto	solido cristallino bianco
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$\Delta_f G^0$ (kJ·mol ⁻¹)	-856,3
S_m^0 (J·K ⁻¹ ·mol ⁻¹)	41,5
$C_{p,m}^0$ (J·K ⁻¹ ·mol ⁻¹)	44,4

SiO₂

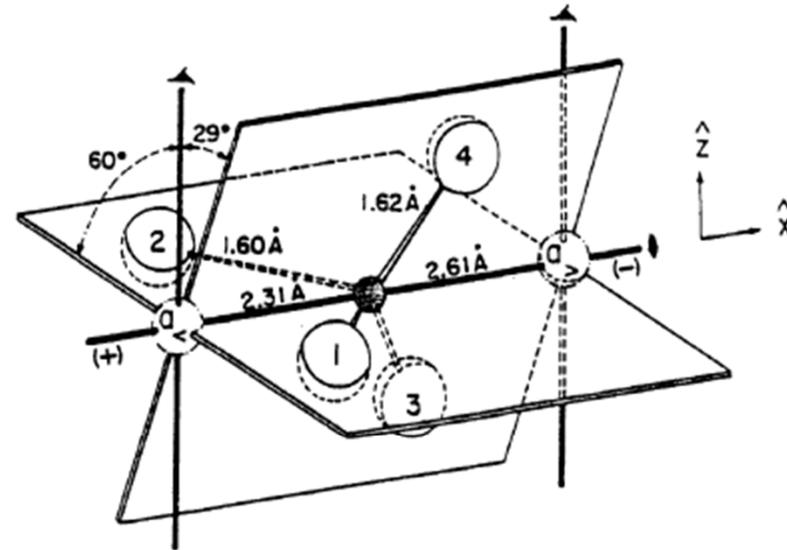


Figure 2 – Details of a SiO₄ tetrahedron in right α -quartz (See Fig. 1). Symbols $a_{<}$ and $a_{>}$ locate possible sites for an interstitial atom/ion in the middle of a large c -axis channel at its intersection with the two-fold axis $\mathbf{a}_1 = x$ -axis. Symbols \pm give the sign of the electrical charge developed on \mathbf{a}_1 when the crystal is compressed along this direction (- charge on + side of \mathbf{a}_1). Reproduced from Fig. 7 of [6].

SiO₂

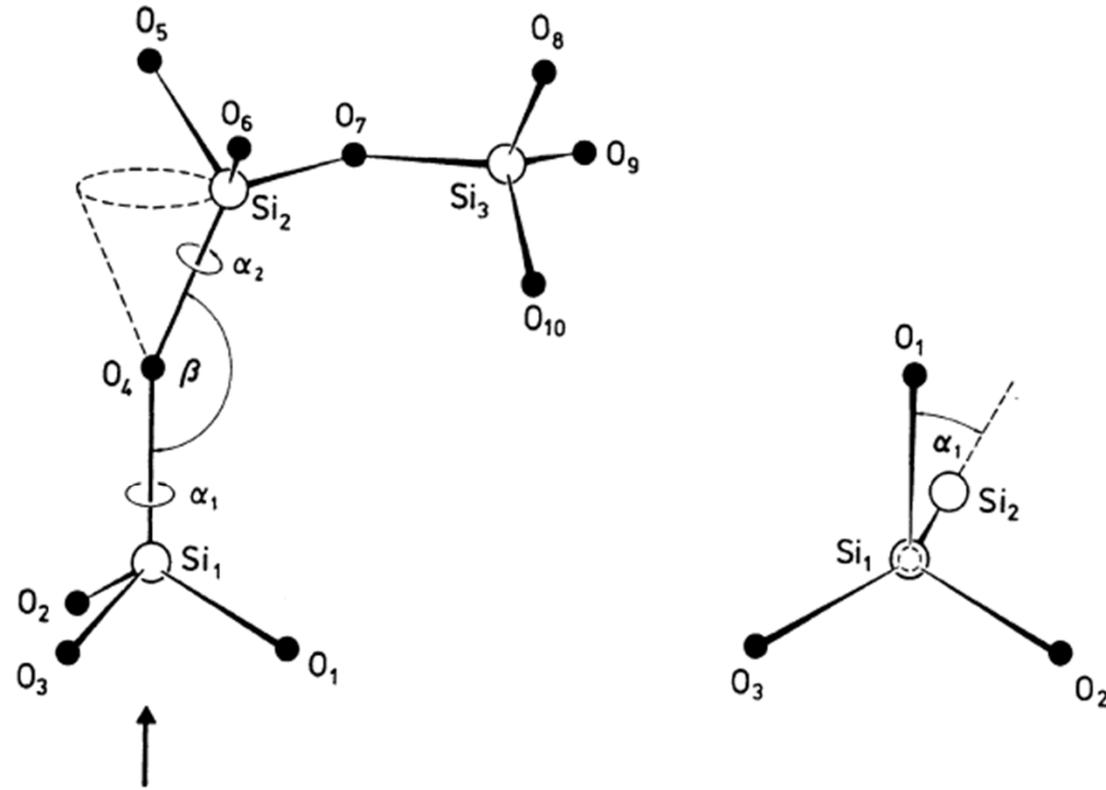


Figure 2. Definition of the bond angle, β , and the torsion angles, α and α_2 , for vitreous SiO₂.

SiO₂

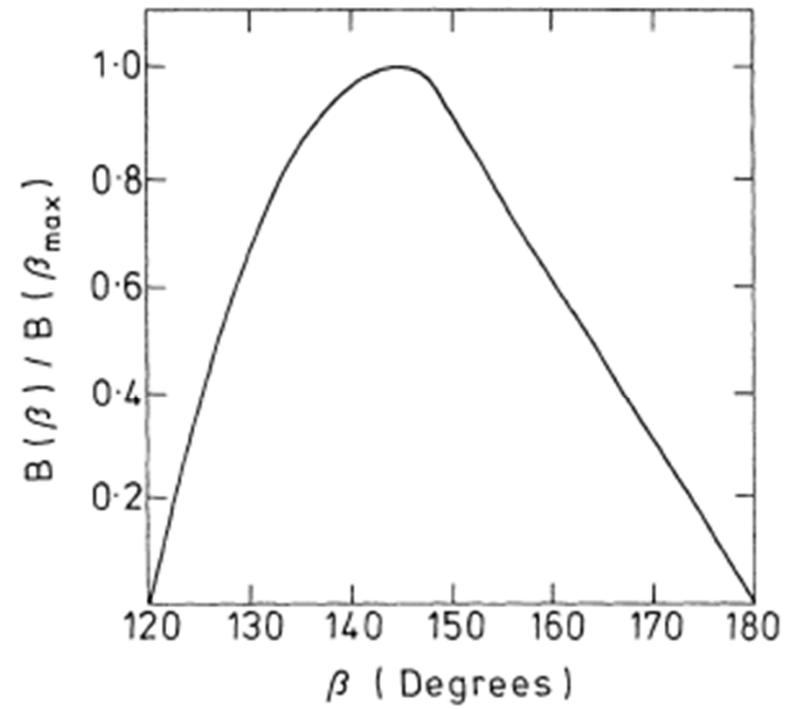


Figure 9. The Si-O-Si bond angle distribution for vitreous SiO₂, as determined by Mozzi and Warren [16].

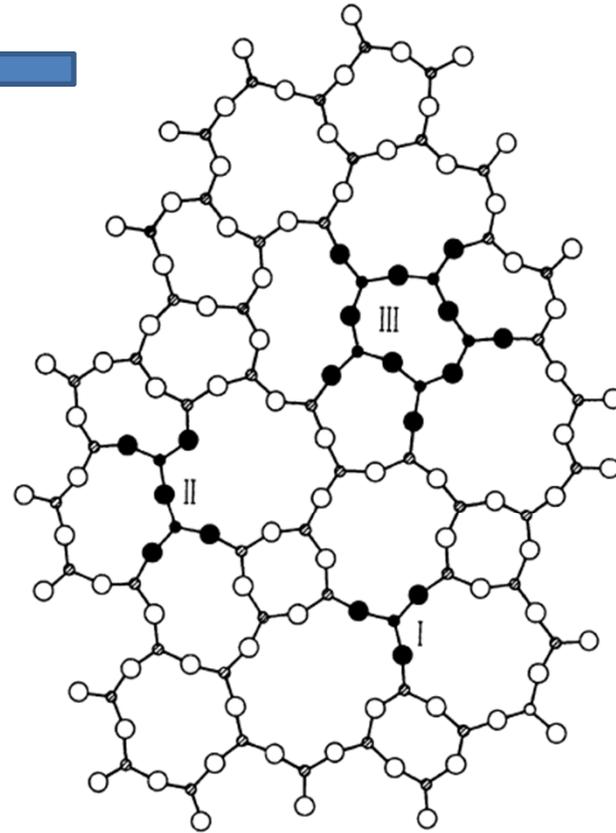


Figure 1. Zachariasen's original random network diagram (retraced) for a glass of composition A_2O_3 [8], with structural units shaded to indicate range I, II and III order. Small atoms, A and large atoms, O. Note the regularity of the AO_3 structural units.

SiO₂

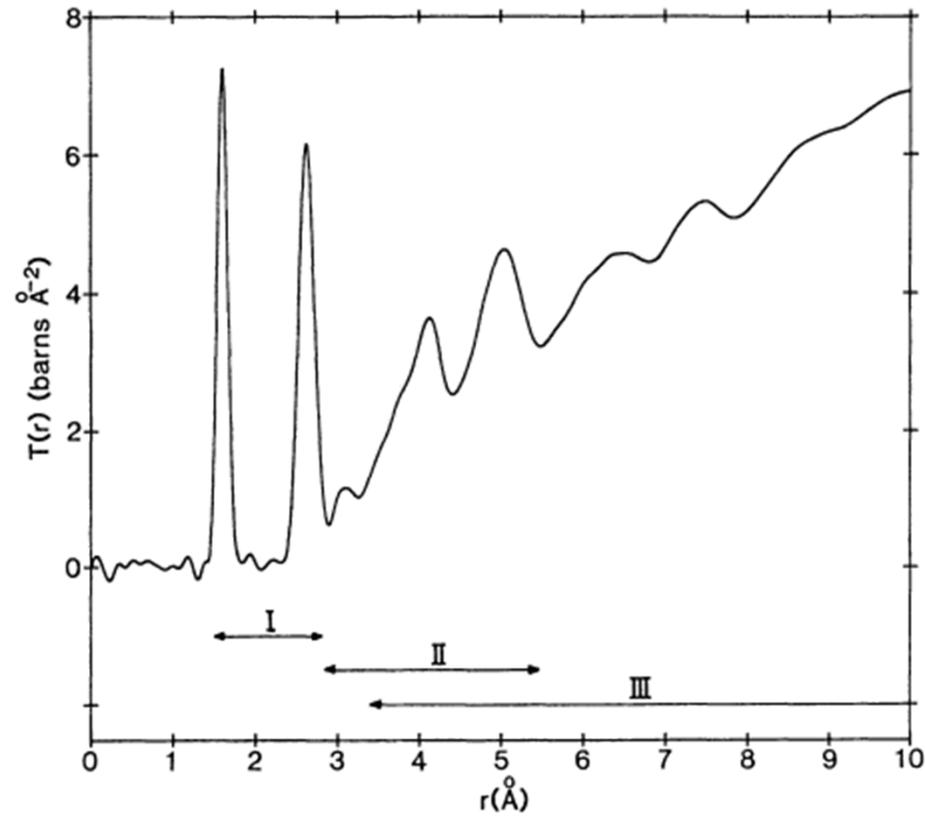
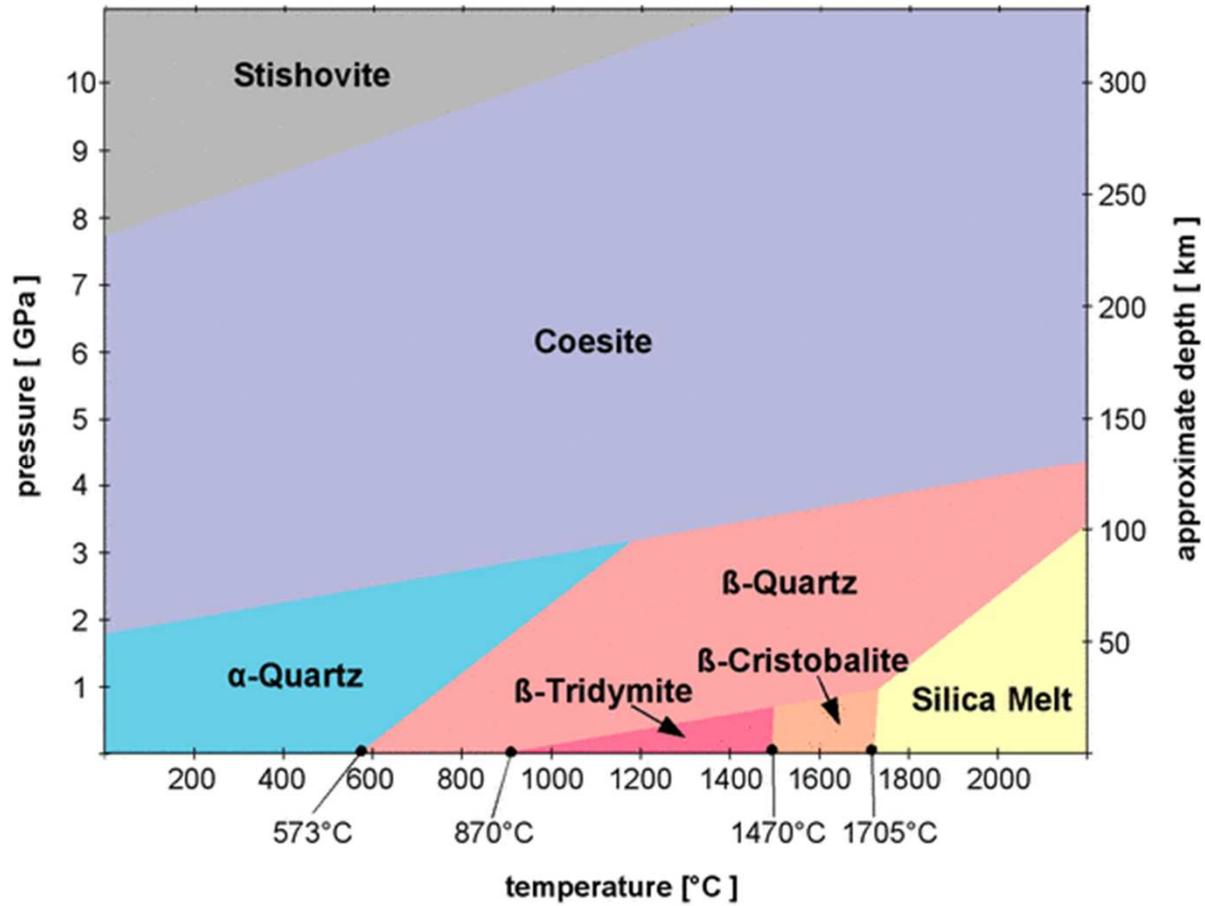


Figure 4. The neutron correlation function, $T^N(r)$, for vitreous SiO_2 ($Q_{max} = 45.2 \text{ \AA}^{-1}$) [17,18], showing the extent of the contributions from range I, II and III order.

Polymorph/Regrowth	Avg. Si-O-Si Angle θ , $^{\circ}$	Avg. Ring Size	Avg. Local Cluster Size	Density, $\times 10^3$ kg/m 3
HP-Tridymite	149.5	6	27	2.18*
β -Cristobalite	148.0	6	29	2.21*
α -Cristobalite	145.3	6	29	2.33*
Keatite	154.1	6.9	39	2.50*
α -Moganite	138.5	7.4	41	2.62*
α -Quartz	143.6	7.7	63	2.65*
β -Quartz	150.9	7.7	63	2.77*
Coesite	150.8	10.0	78	3.01*
Vitreous Silica	145	~ 6	?	2.21*

Polymorph	Stability Regime	Density	Primitive Ring Content
Cristobalite	high temperature (1743-2001 K)	α 2.33	12 6-rings
		β 2.21	
Tridymite	high temperature (1140-1743 K)	HP 2.18	12 6-rings
		MC 2.26	
Vitreous Silica	high temperature ($T_g \sim 1333$ K)	2.21	$n \approx 6?$

In "Defects in SiO $_2$ and related dielectrics: Science and Techn. "
Ed. G.Pacchioni, L.Skuja, D.L. Griscom, Kluwer 2000



C. Koike et al. The Astroph. Journ. (2013) 778, 60

<http://www.quartzpage.de>

I difetti di punto

Invarianza delle proprietà fisiche dei materiali durante il loro utilizzo:

Esposizione alla radiazione ionizzante (UV, raggi X, raggi γ)

Applicazioni in ambienti radioattivi o in applicazioni spaziali (lenti, fibre, strati isolanti nei MOS)

Investigazione delle strutture microscopiche che danno luogo a specifiche proprietà:

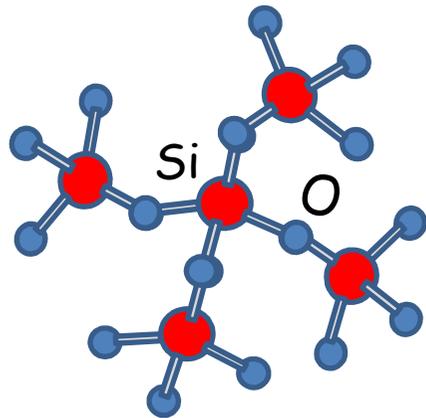
Sensibilità-resistenza alla radiazione

Centri di colore per applicazioni fotoniche: FBG, Laser, dispositivi non lineari

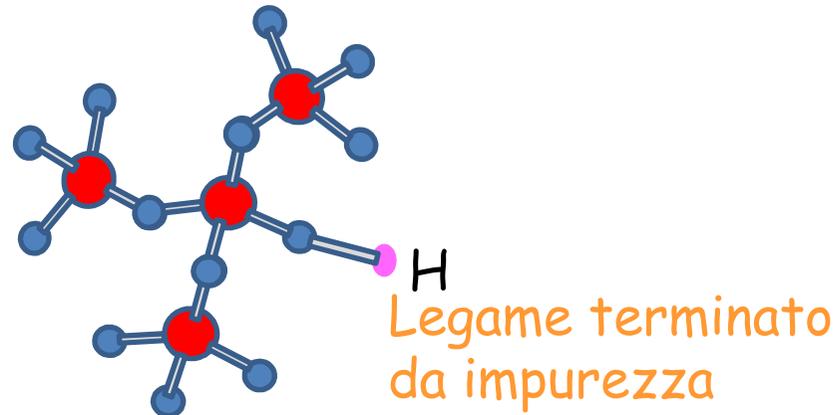
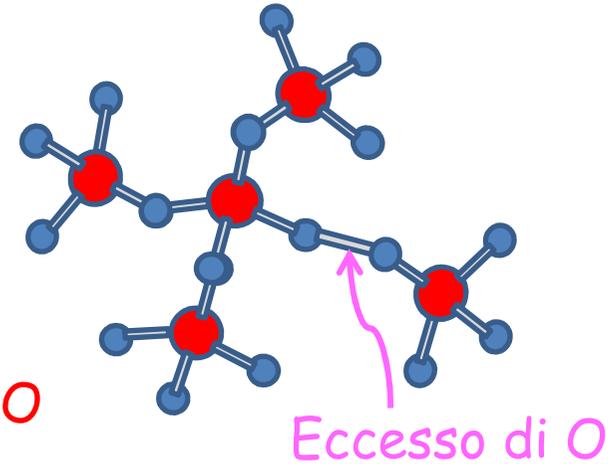
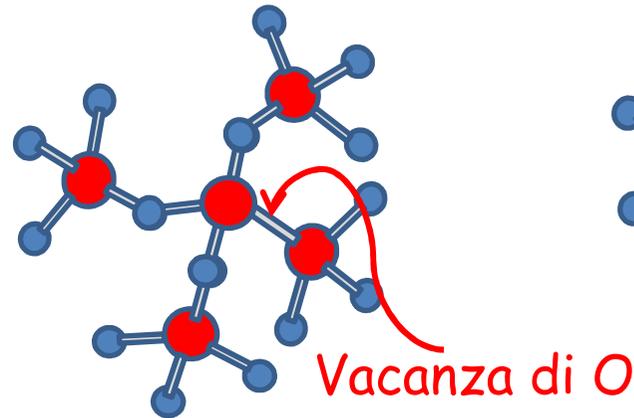
Difetti di punto in applicazioni elettroniche

I difetti di punto

Difetto di punto = distorsione a livello atomico della silice



Frammento regolare



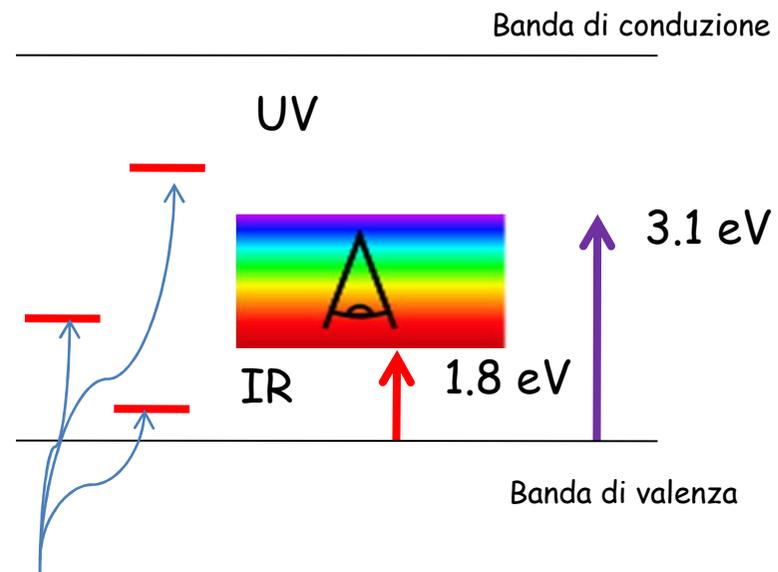
I difetti di punto

Difetto di punto = comparsa di livelli energetici nella regione di energie proibite

Effetti causati:

Perdita di trasparenza con assorbimento ed emissione di luce

Possibilità di intrappolare cariche con modifica delle proprietà elettriche

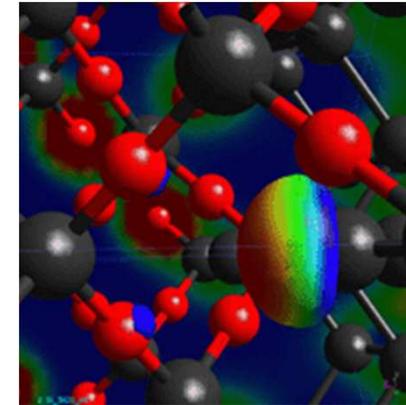
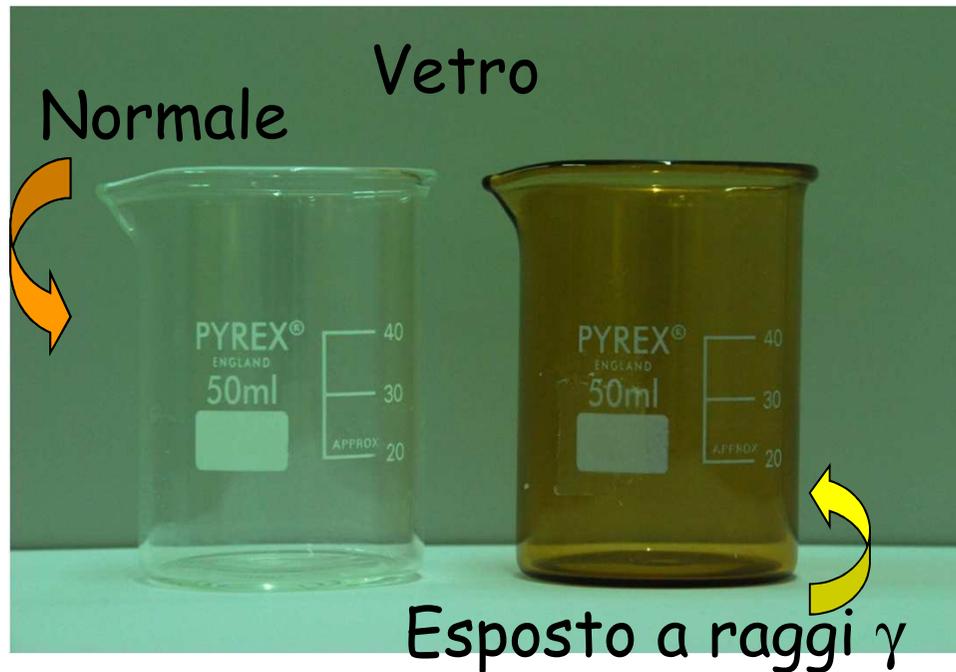


livelli energetici dovuti ai difetti

Studio "microscopico" del SiO_2

Effetti della radiazione ionizzante

(Laser, raggi X, raggi γ , raggi β ,...)
generazione di centri di colore



Determinazione delle
strutture atomiche e dei
processi di formazione dei
centri di colore

Tecniche: Spettroscopia Ottica

Absorption, Nonradiative Relaxation and Luminescence
Making **heat** and **1x red** out of **1x blue**

