Excitons, Raman spectroscopy

Frenkel Excitons

A Frenkel exciton is localized on an atom or molecule in a crystal.

The band gap of solid krypton is 11.7 eV. Lowest atomic transition in the solid is 10.17 eV.

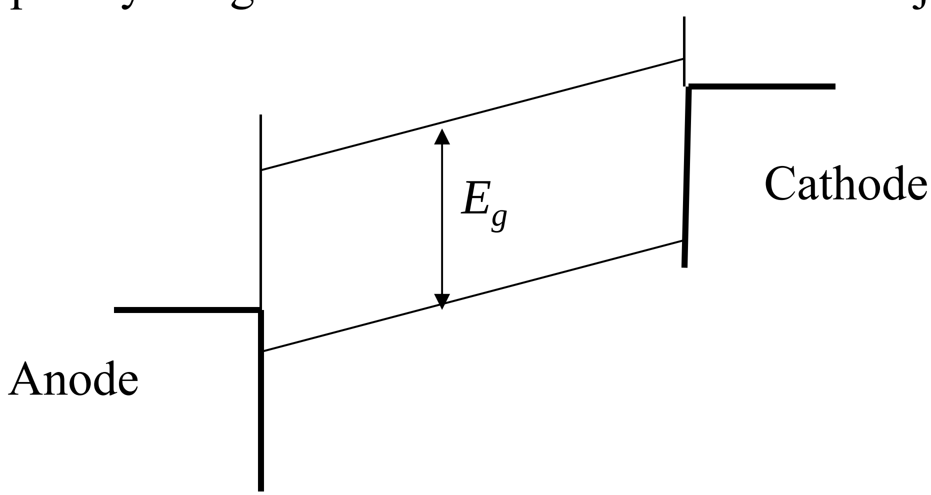
Excitons transport energy but not charge. Frenkel excitons are occur in organic solar cells, organic light emitting diodes, and photosynthesis.

OLEDs

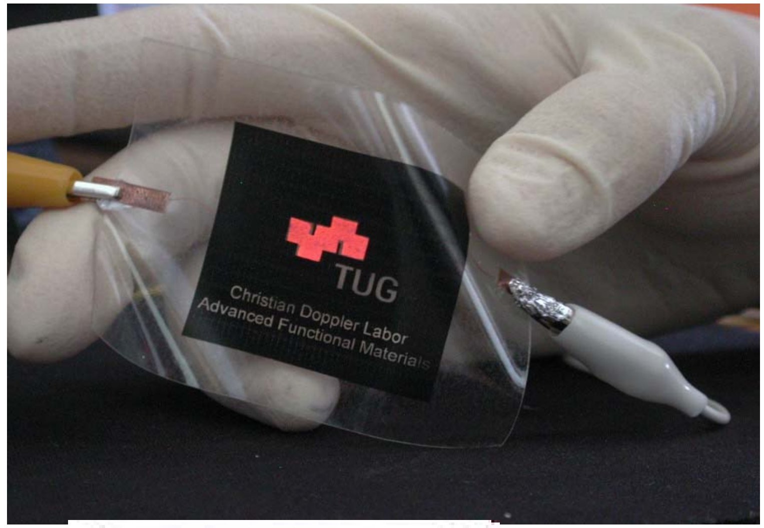
Aluminum cathode
Electron transport layer
Emission layer
Hole transport layer
ITO anode
Glass

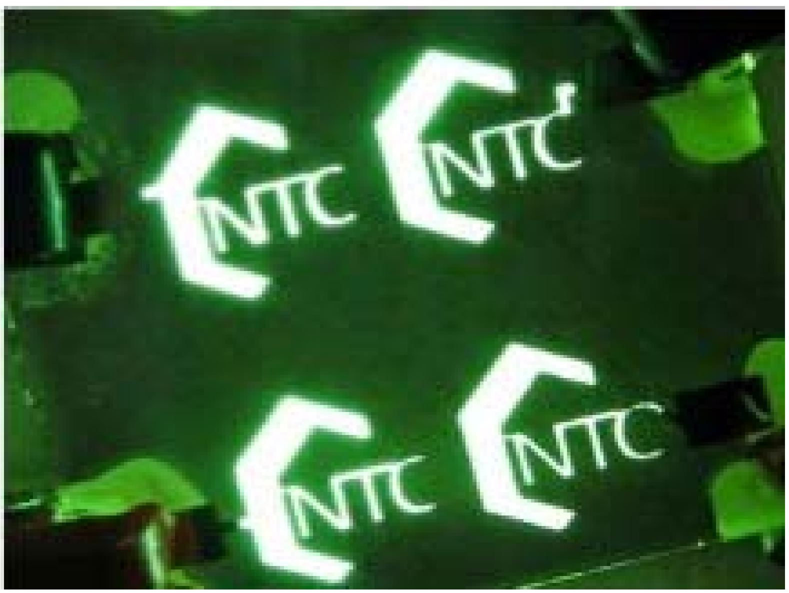
Cathode is typically a low work function material Al, Ca - injects electrons

Anode is typically a high work function material ITO - injects holes



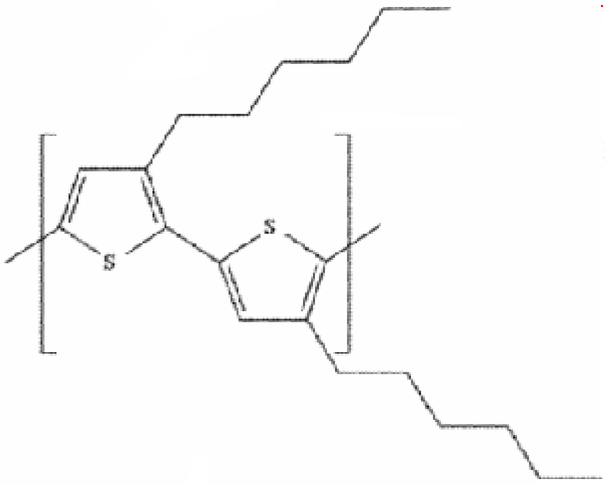
OLEDs



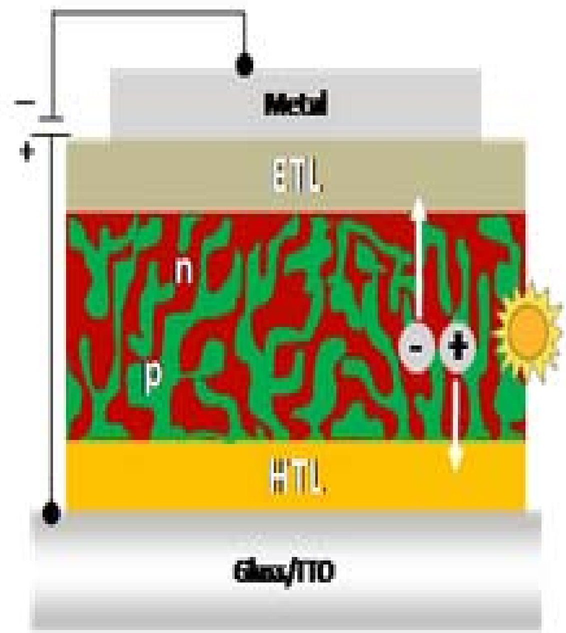


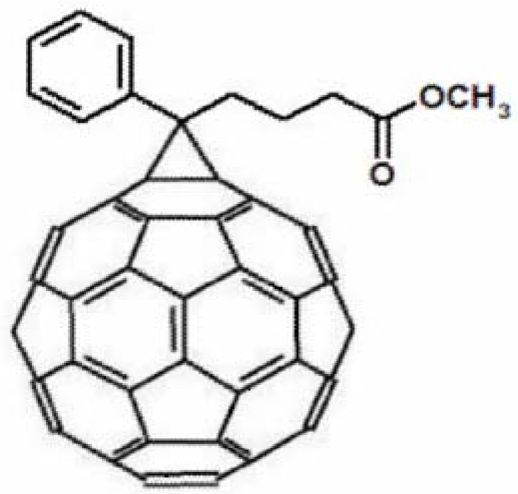
Galaxy Tab

Organic solar cells



P3HT donor



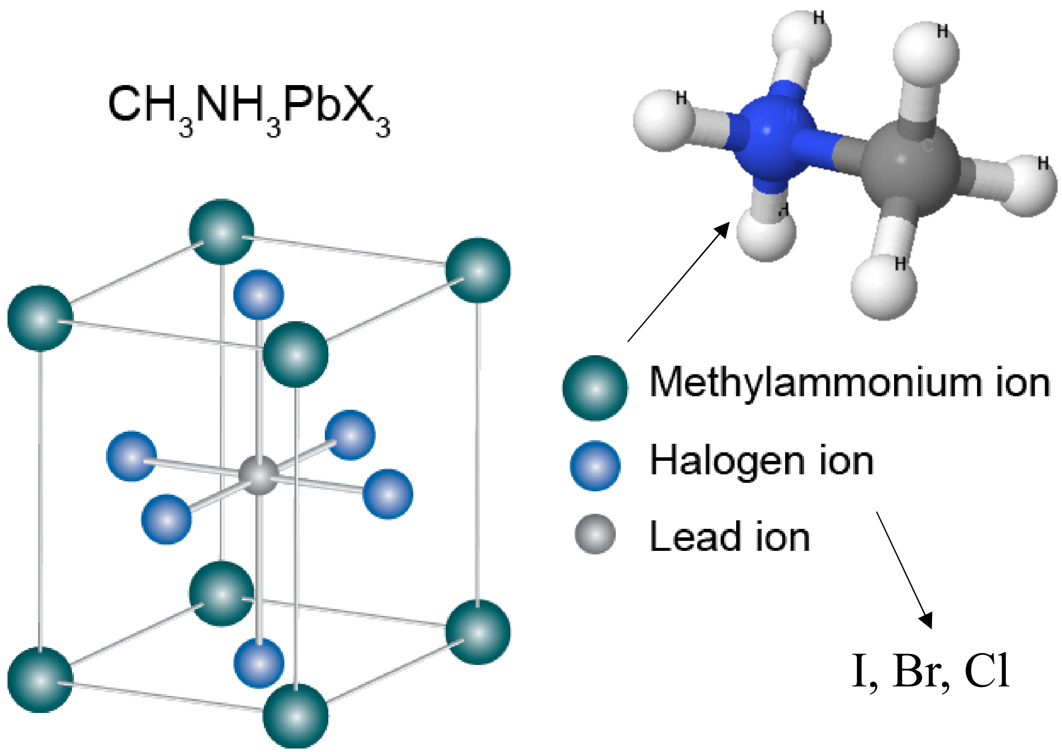


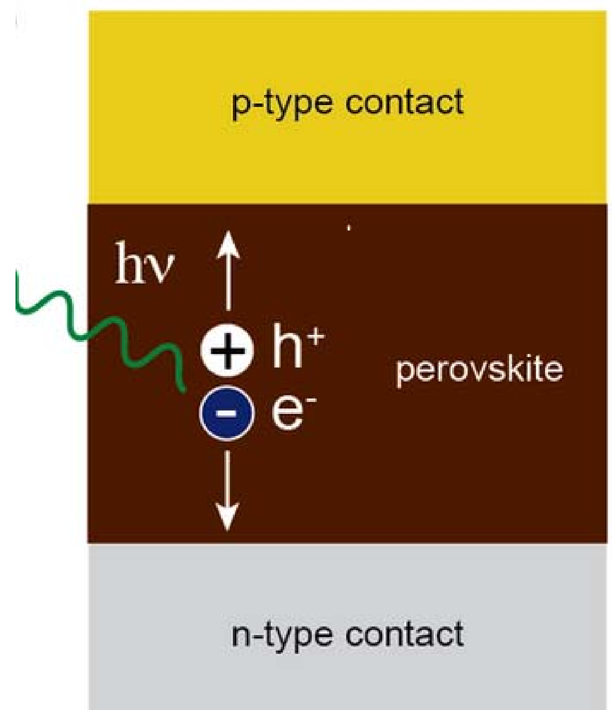
PCBM acceptor

Excitons in polymers: a monomer is in an excited states and this moves down the chain.

https://www.uni-ulm.de/nawi/nawi-oc2/forschung/ag-organische-halbleiter-und-farbstoffe-fuer-die-photovoltaik.html?print=1

Perovskite solar cells





Efficiency ~ 22%

https://en.wikipedia.org/wiki/Perovskite_solar_cell

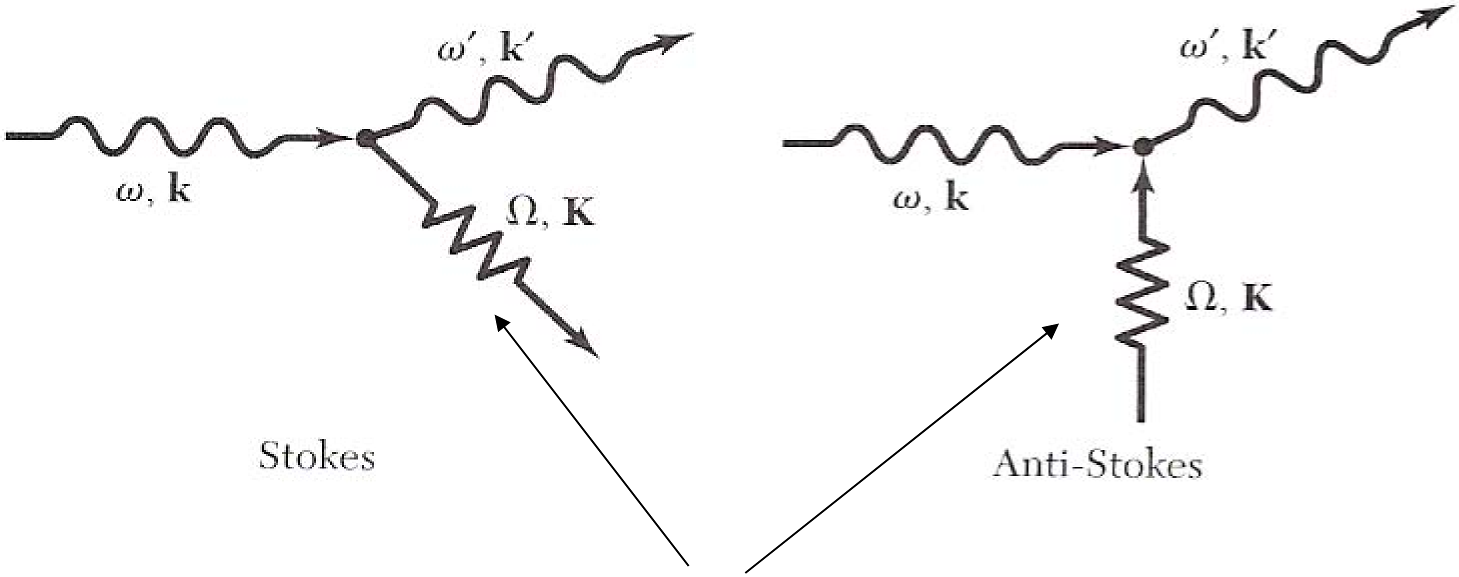
Raman Spectroscopy

C. V. Raman

Inelastic light scattering

$$\omega = \omega' \pm \Omega$$

$$\vec{k} = \vec{k}' \pm \vec{K} \pm \vec{G}$$



Phonons, magnons, plasmons, polaritons, excitons

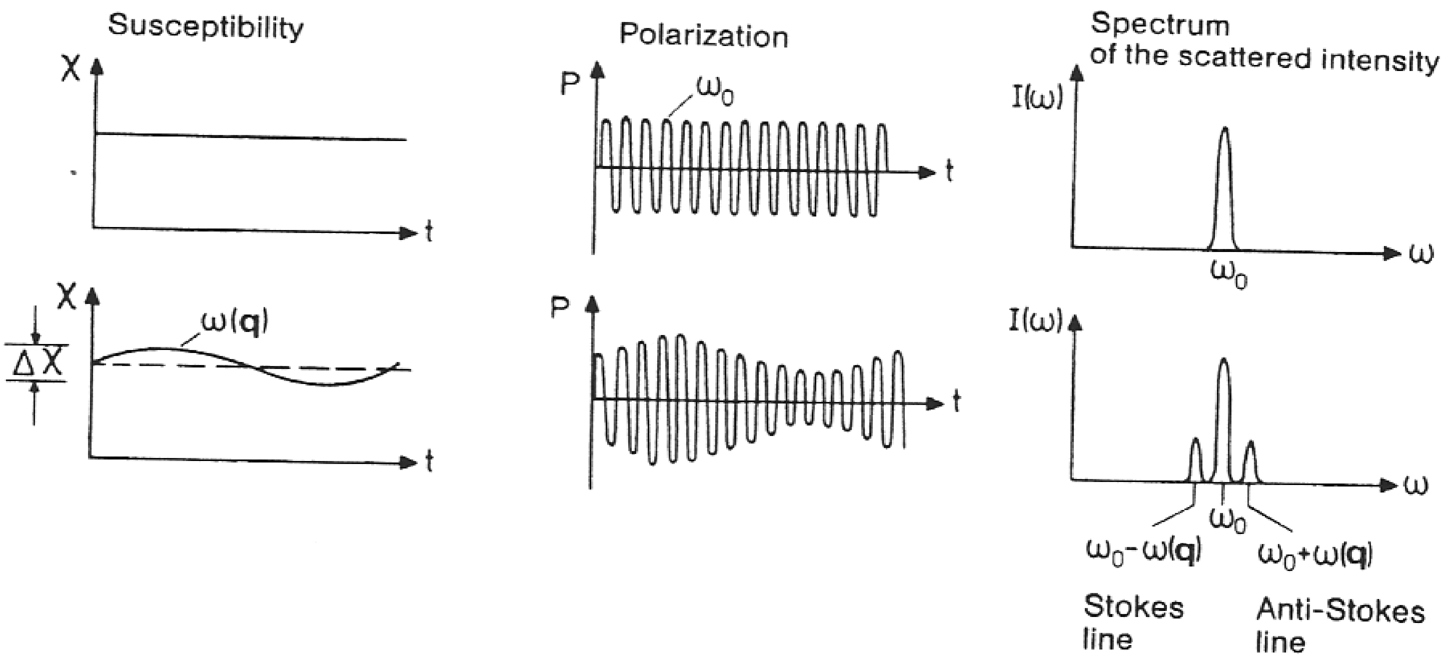
$$\vec{K} \approx 0$$

Raman Spectroscopy

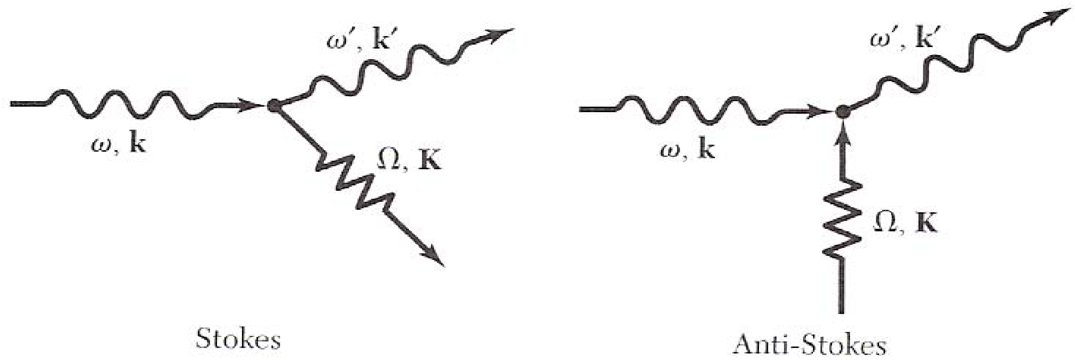
$$\chi = \chi_0 + \frac{\partial \chi}{\partial X} X \cos(\Omega t)$$

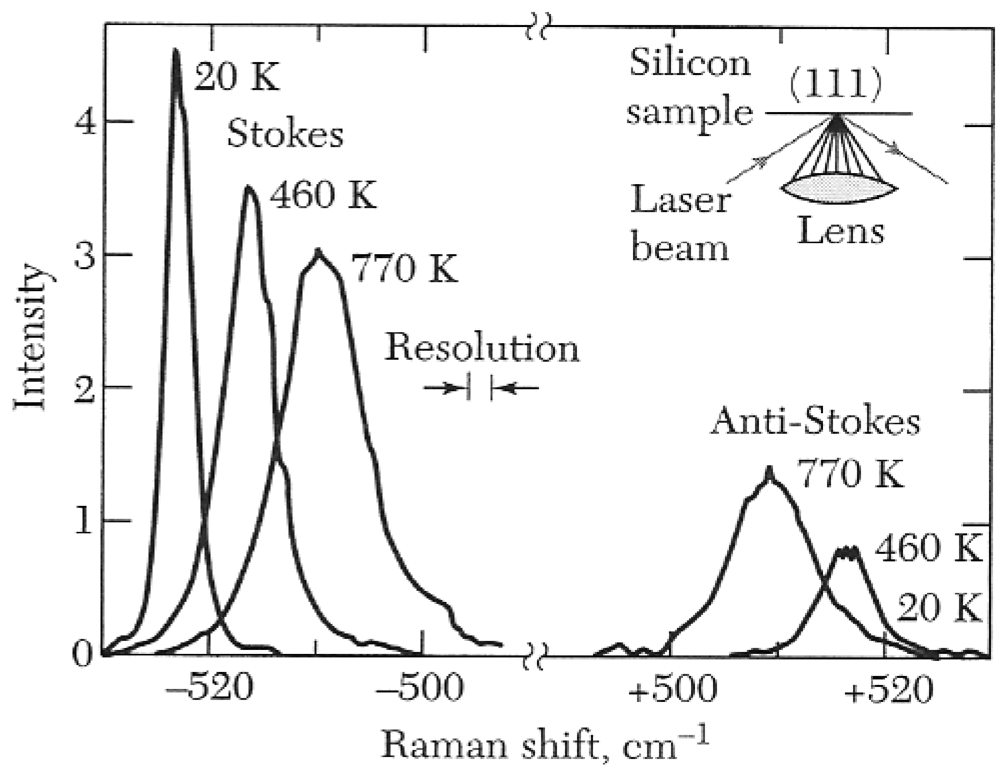
$$\vec{P} = \varepsilon_0 \chi \vec{E} \cos(\omega t) + \varepsilon_0 \frac{\partial \chi}{\partial X} X \cos(\Omega t) \vec{E} \cos(\omega t)$$

There are components of the polarization that oscillate at $\omega \pm \Omega$.



Raman Spectroscopy





Stokes:

$$I(\omega - \Omega) \propto n_k + 1$$

anti-Stokes:

$$I(\omega + \Omega) \propto n_k$$

Raman spectroscopy

PHYSICAL REVIEW B, VOLUME 64, 035204

Vacancy-hydrogen defects in silicon studied by Raman spectroscopy

E. V. Lavrov* and J. Weber

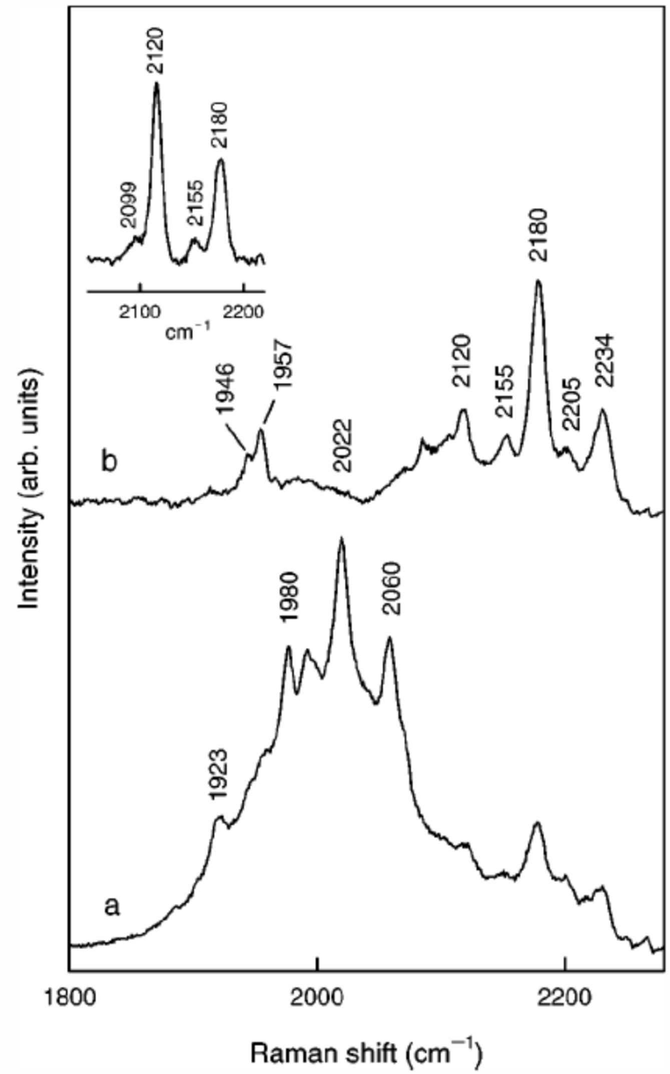


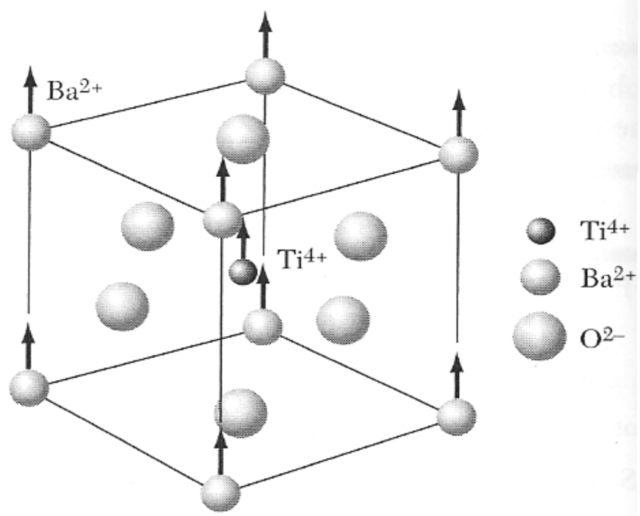
FIG. 1. Raman spectra measured at room temperature on the H_2-implanted sample: (a) as-implanted sample, (b) after annealing at 400 °C for 2 min. Spectra are offset vertically for clarity.

Ferroelectricity

Ferroelectricity

ABX$_3$

Perovskites

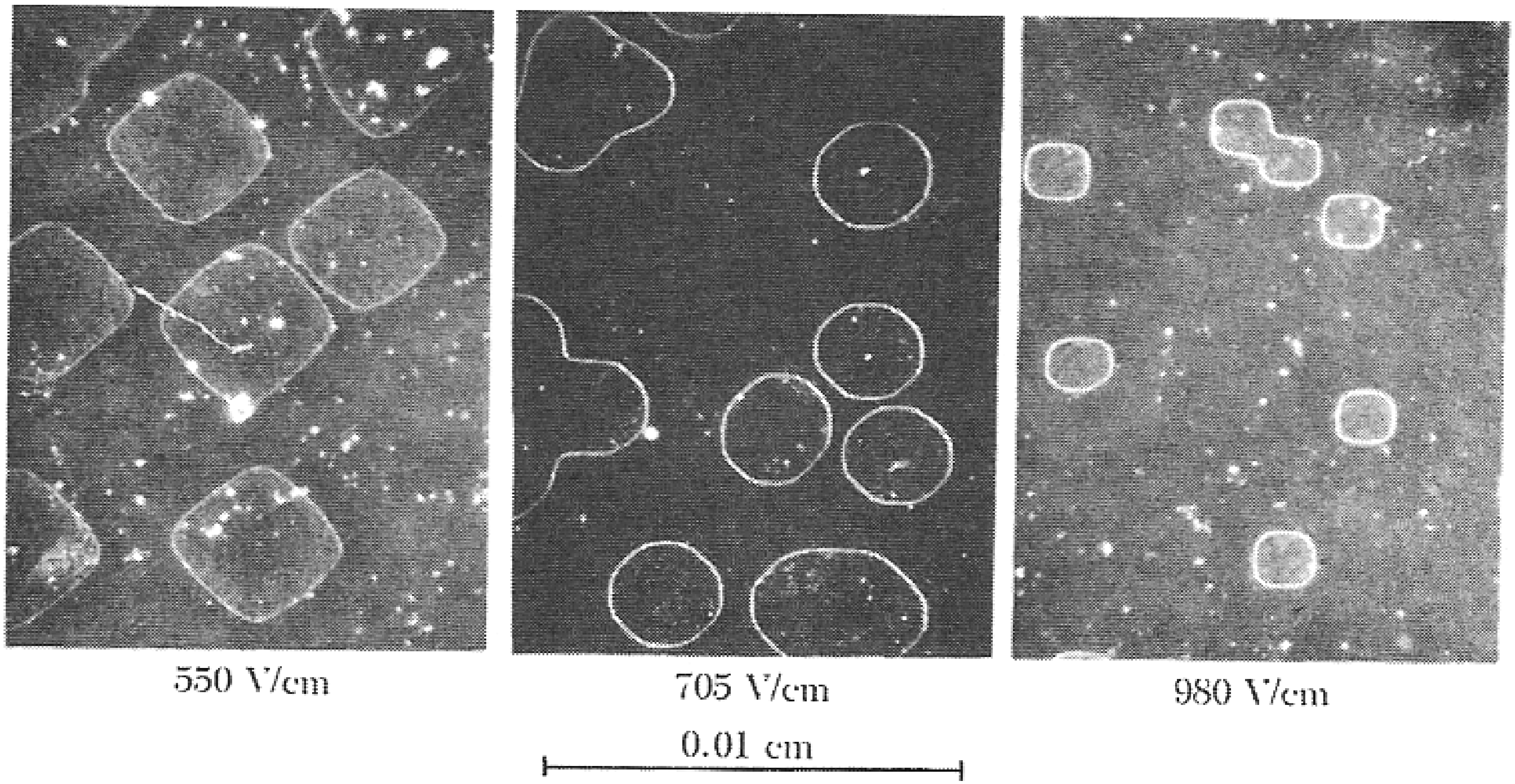


Spontaneous polarization
Analogous to ferromagnetism
Structural phase transition
T_c is transition temperature

Electric field inside the material,
is not conducting

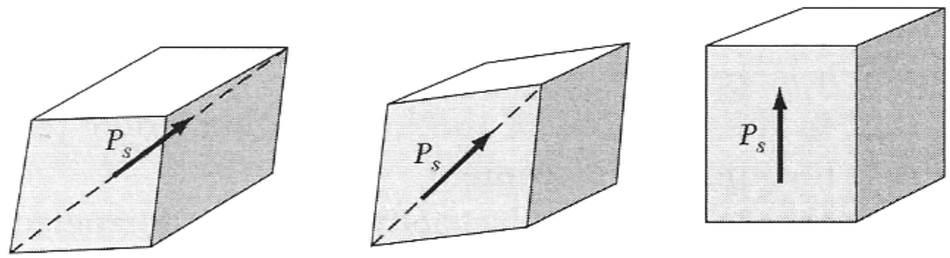
		T_c, in K	P_s, in μC cm^{-2}, at T K	
KDP type	KH_2PO_4	123	4.75	[96]
	KD_2PO_4	213	4.83	[180]
	RbH_2PO_4	147	5.6	[90]
	KH_2AsO_4	97	5.0	[78]
	GeTe	670	—	—
TGS type	Tri-glycine sulfate	322	2.8	[29]
	Tri-glycine selenate	295	3.2	[283]
Perovskites	$BaTiO_3$	408	26.0	[296]
	$KNbO_3$	708	30.0	[523]
	$PbTiO_3$	765	>50	[296]
	$LiTaO_3$	938	50	
	$LiNbO_3$	1480	71	[296]

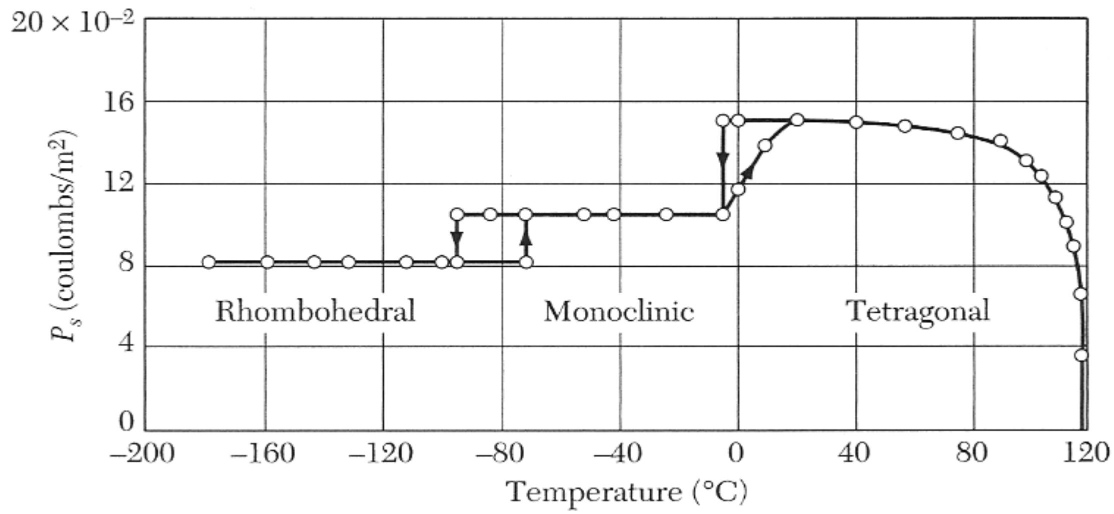
Ferroelectric domains

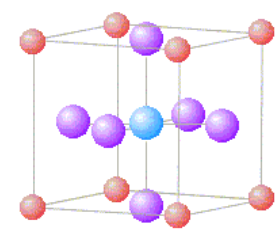


Increasing the electric field polarizes the material.

$BaTiO_3$







cubic (contains i => no spontaneous P)

Can be used to make nonvolatile memory