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SPRING COLLEGE ON AMORPHOUS SOLIDS
AND THE LIQUID STATE

14 April - 18 June 1982

DEFECTS AND DEFECT MODELS
(Part I)

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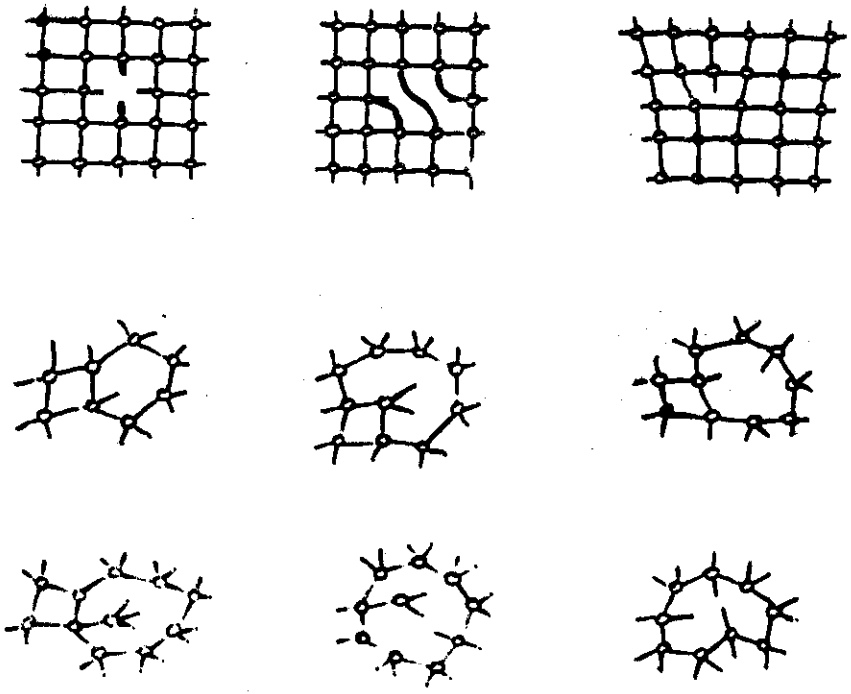
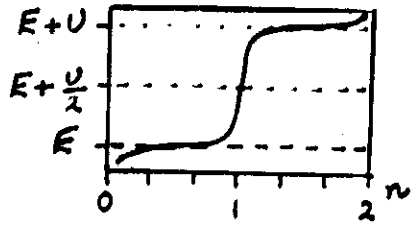


VARIATION OF E_F WITH n FOR $\pm U$ DEFECTS

n = average number of electrons per defect site

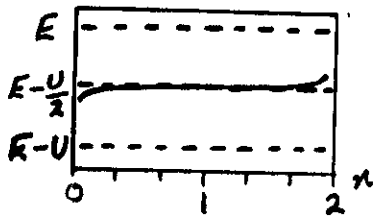
POSITIVE U



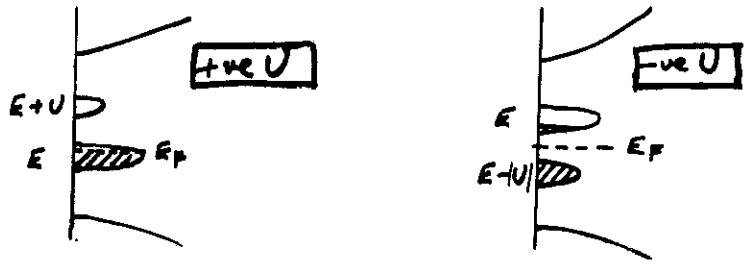
$$E_F = E - kT \ln\{2|(n-1)|/1-|(n-1)|\} \qquad 0<n<1$$

$$E_F = E + U - kT \ln\{2|(n-1)|/1-|(n-1)|\} \qquad 1<n<2$$

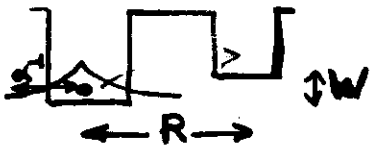
NEGATIVE U



$$E_F = E - |U|/2 - (kT/2)\ln[(2/n)-1] \qquad 0<n<2$$

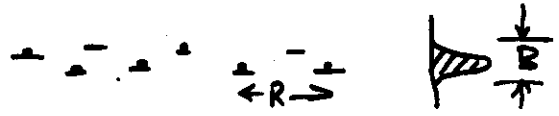


HOPPING CONDUCTION



Frequency $\nu = \nu_0 \exp(-W/kT) \exp(-2\alpha R)$

phonon-assisted quantum mechanical tunnelling



$4/3\pi R^3 = 1/N$

$\mu = eD/kT$ (Einstein relation)

$D = \frac{1}{6}\nu R^2$ (diffusion-like motion)

$$\mu = \frac{eR^2}{6kT}\nu_0 \exp(-W/kT)\exp(-2\alpha R)$$

NEAREST-NEIGHBOUR HOPPING CONDUCTION

$\sigma = ne\mu = \underline{N(E_F)kTe\mu}$

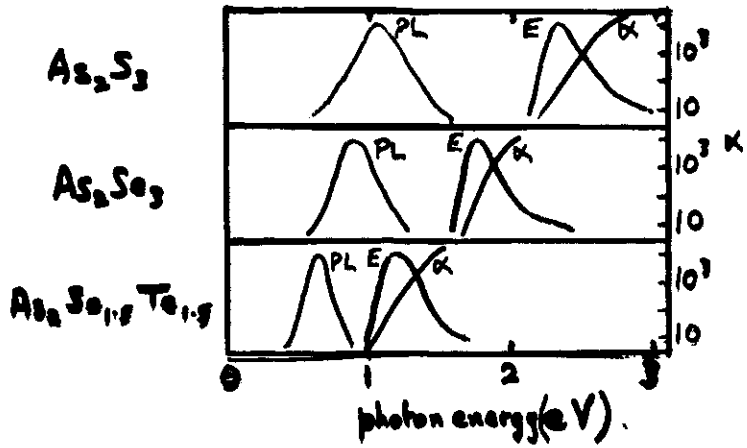
$= \underline{N(E_F)\ldots}\ \nu_0 \exp(\ldots)\exp(\ldots)$

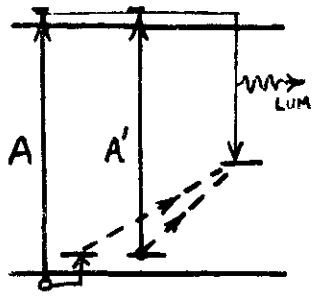
$(\ln\sigma \propto 1/T)$

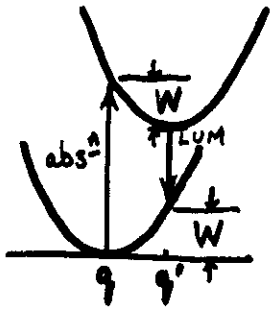
MAX VALUE $\sim \nu_{ph} \sim 10^{12}\,s^{-1}$

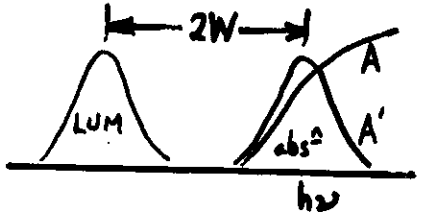
cf. For extended states $\nu \sim km/R^2 \sim 10^{15}\,s^{-1}$

$\mu_{ext} = \frac{1}{6}\frac{k}{m}\frac{e}{kT} \sim 6\ cm^2 V^{-1} s^{-1}$









DEFECTS IN CHALCOGENIDES

Consider a dangling bond (chain end) in Se.
It can contain 0, 1, or 2 electrons

D^+ (positive, no spin) D° (neutral, spin) D^- (negative, no spin)

$D^+ + e\ (+E_1) \rightarrow D^\circ$ $D^\circ + e\ (+E_2) \rightarrow D^-$

Normally $E_2 > E_1$ $E_2 - E_1 = U$ = correlation energy

With structural rearrangements, however, possible for

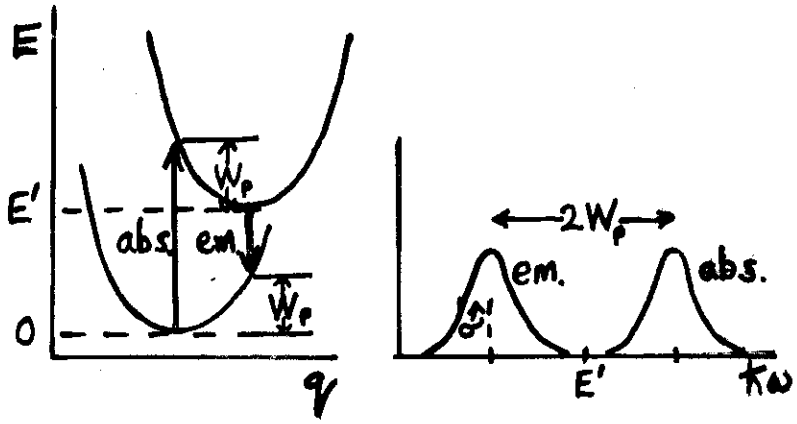
$E_2 < E_1$ $E_2 - E_1 = U_{eff}$ (negative)

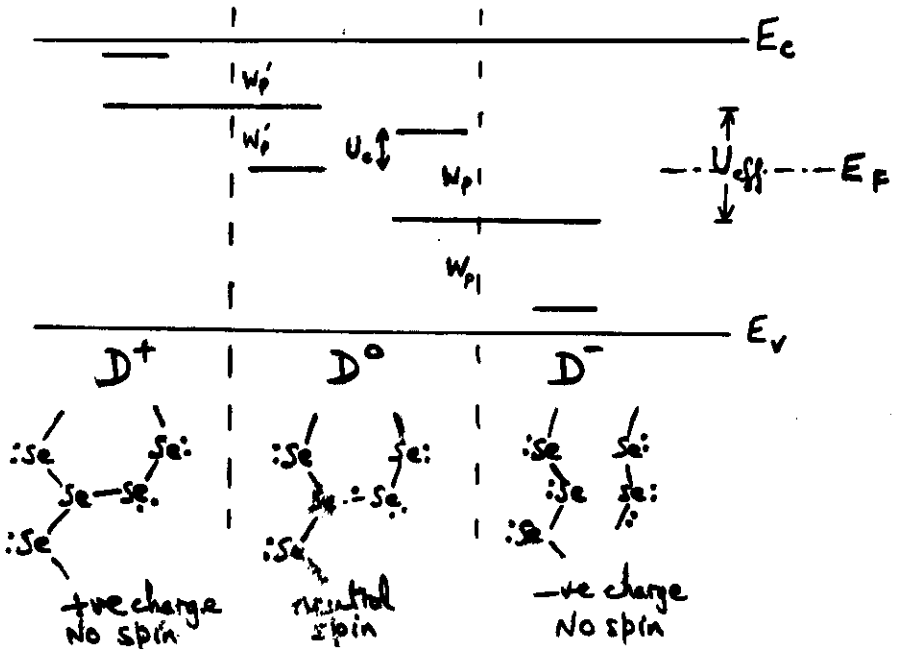
$D^+(+E_1) - D^\circ(-E_2) \rightarrow D^\circ - D^-$

ie $2D^\circ \rightarrow D^+ + D^- + (E_1 - E_2)$

EXOTHERMIC REACTION – spontaneous creation of charged, spinless defects

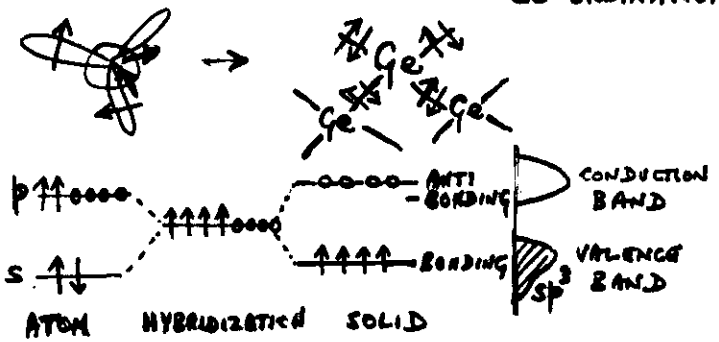
configurational coordinate diagram



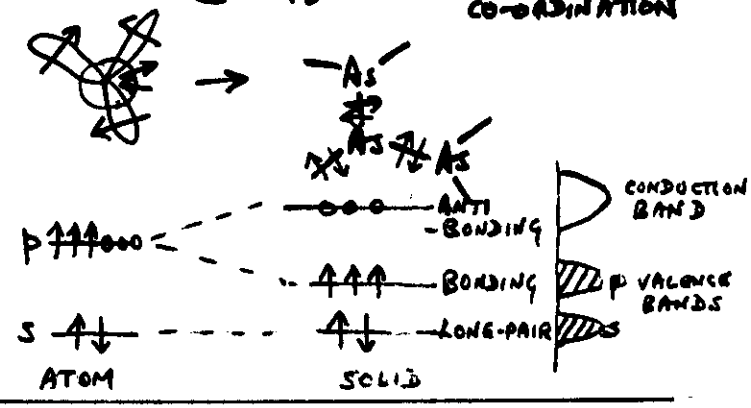


CHEMICAL BONDING

Ge (Si) s^2p^2 forms 4 sp^3 hybridized orbitals
@ 109° 28′ TETRAHEDRAL CO-ORDINATION



As (Sb, P) s^2p^3 forms 3 p orbitals
@ ~ 98° TRIGONAL CO-ORDINATION



Se (Te) s^2p^4 forms 2 p bonding orbitals @ 105°

2 lone-pair orbitals