Electronic structure of C_{60}: photoelectron spectroscopic Study

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Introduction

Electronic Structure of C_{60} – HMO treatment

UPS of C_{60} , C^{-}_{60}

$K_x C_{60}$ thin films

Conclusions

Introduction

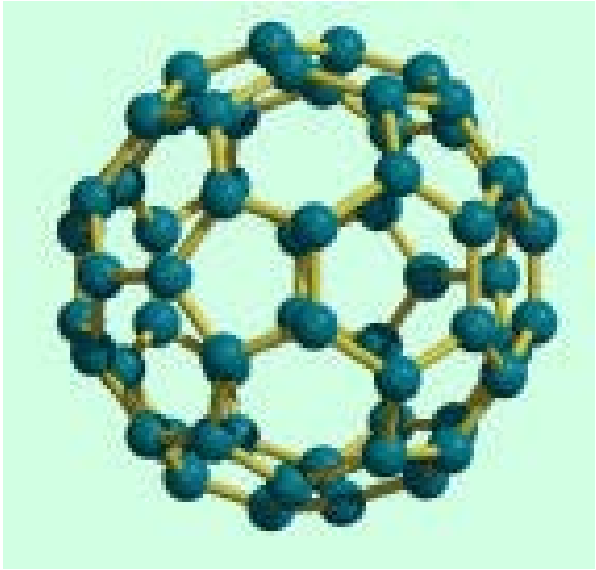
Discovered in 1985 by David Kroto and R.E.Smalley during mass spectroscopic studies of carbon clusters

Named in the honour of american architect Richard Buckminister Fuller as Buckministerfullerene

Naturally occuring deposit - shungite (Russia)

Crystal Structure - fcc

High symmetry- I_h



Electronic Structure of C_{60} – HMO treatment

Huckel molecular orbital theory for non-planar conjugated organic molecules has been applied to study the electronic structure.

C_{60} was found to be non-alternant molecule.

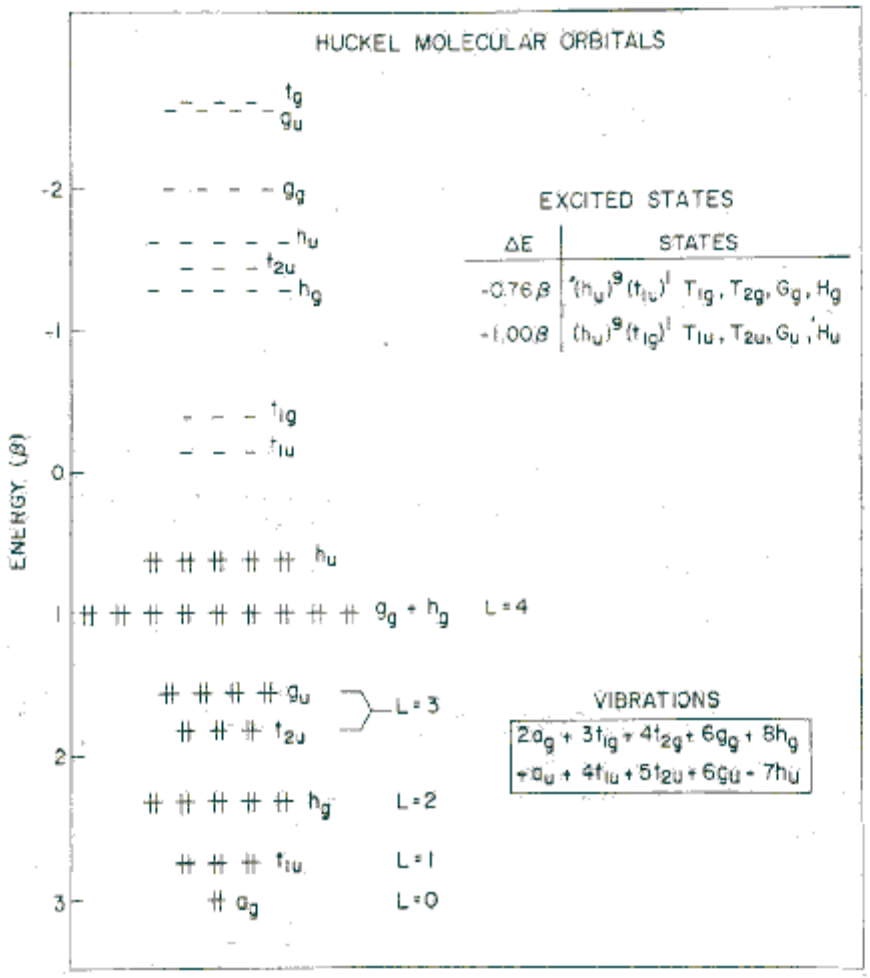
All carbon atoms are sp^2 hybridised.

Charge densities on all carbon atoms are equal.

There are 20 six-membered rings and 12 five-membered rings

There is an asymmetric distribution of HOMO and LUMO molecular orbitals about zero of energy

Planar HMO treatment



HMO energy level diagram for C_{60} (unscaled β, see text).

Photoemission Study-Electronic Structure of C_{60}

Photoemission is a powerful tool for investigating the electronic structure of solids.

The unsolved problems are

1. To observe fine structure in the electronic distribution predicted by calculation

2. To find the degree to which structural phase transitions of C_{60} effect the electronic structure

UPS of C^-_{60}

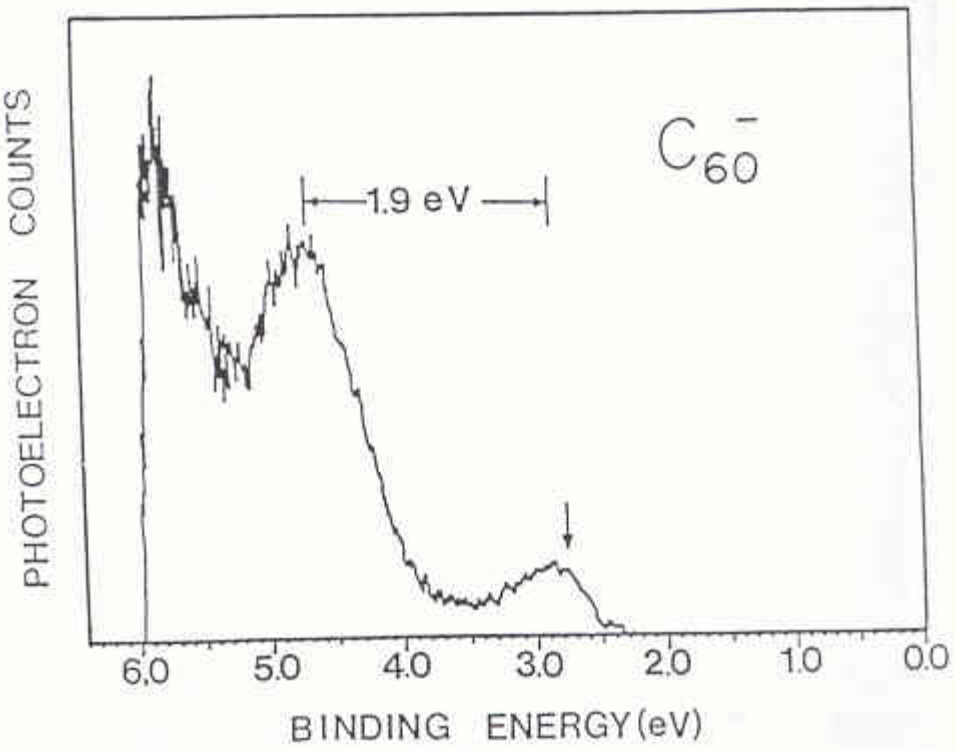
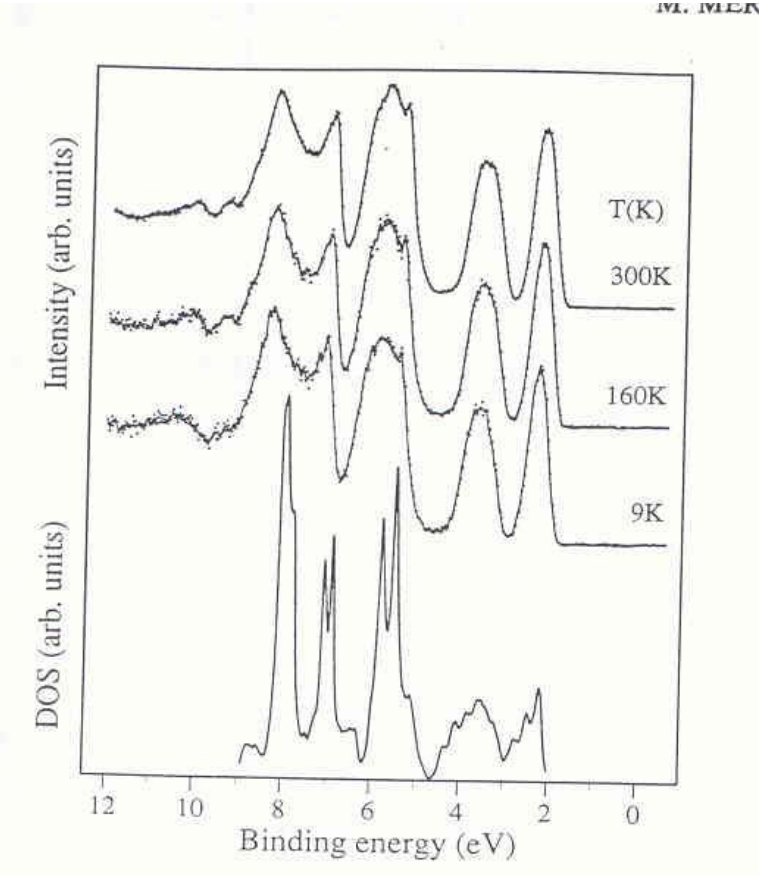


Fig. 3. Expanded view of the ultraviolet photoelectron spectrum of C_{60}^- (Buckminsterfullerene) taken with an ArF excimer laser.

Electron affinity = 2.8 eV

HOMO-LUMO gap = 1.9 eV

Temperature dependent high-resolution UPS spectra of pure C_{60}



Π- derived HOMO (h_{1u}), HOMO-1 (h_g, g_g), HOMO-2 (t_{2u}, g_u) molecular orbitals

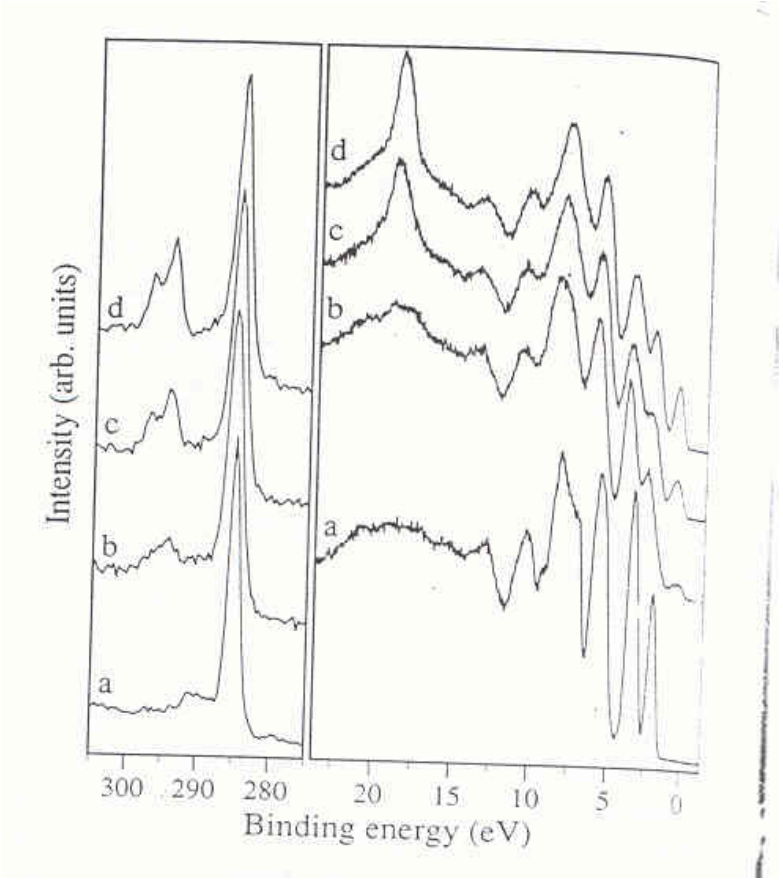
Calculated valence-band DOS (electronic density of states) of unidirectionally oriented C_{60}

$K_x C_{60}$ thin films

C_{60} is a semi conducter

K_3C_{60} is a metal

To study the change in the electronic structure of C_{60} on K doping

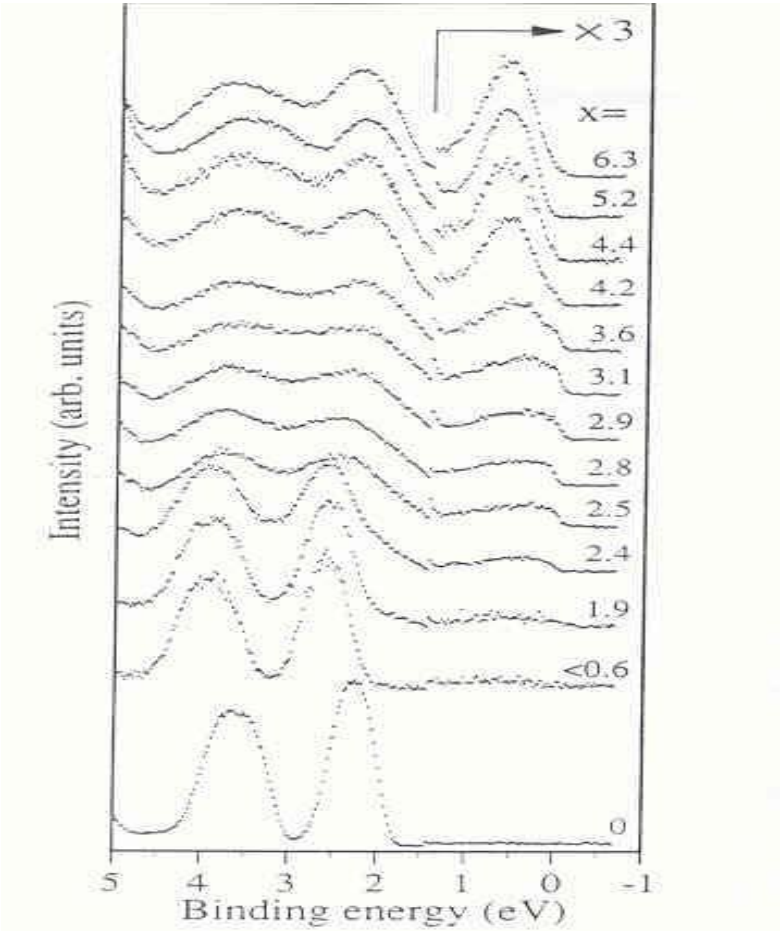


Right side- energy distribution curves (EDC's) of $K_x C_{60}$, X= 0, 2.3, 4.3, 6.3

Left-hand panel: XPS spectra of C 1s and K 2p core levels

Progressive occupation of LUMO as K doping level increases

Room temperature high-resolution photoemission spectra of $K_x C_{60}$



There is a broadening of LUMO and HOMO derived bands

Conclusions

1. The discovery of super conductivity in alkali metal-doped fullerides has prompted the research concerning the electronic properties of these molecules
2. High resolution photoelectron spectroscopy lead to the more accurate determination electron affinity

References

1. Krishnan Raghavachari *et al,* Chemical Physics Letters 125 (1986) 459.
2. Lai-Sheng Wang *et al,* Journal of Chemical Physics 110 (1999) 8217.
3. R.E.Smalley *et al,* Chemical Physics Letters 139 (1987) 233.
4. J.Pink *et al,* Physical Review B 47 (1993) 11470.