Physica C 197 (1992) 251–260
North-Holland

PHYSICA C

Electronic structure of single crystal C_{60}

J. Wu, Z.-X. Shen, D.S. Dessau, R. Cao, D.S. Marshall, P. Pianetta and I. Lindau
Stanford Synchrotron Radiation Laboratory, Stanford, CA 94309, USA

X. Yang, J. Terry, D.M. King and B.O. Wells
Stanford Electronics Laboratories, Stanford, CA 94309, USA

D. Elloway, H.R. Wendt, C.A. Brown, Heinrich Hunziker and M.S. de Vries
IBM Research Division, Almaden Research Center, San Jose, CA 95120-6099, USA

Received 24 April 1992

We report angle-resolved photoemission data from single crystals of C_{60} cleaved in UHV. Unlike the other forms of pure carbon, the valence band spectrum of C_{60} consists of many sharp features that can be essentially accounted for by the quantum chemical calculations describing individual molecules. This suggests that the electronic structure of solid C_{60} is mainly determined by the bonding interactions within the individual molecules. We also observe remarkable intensity modulations of the photoemission features as a function of photon energy, suggesting strong final state effects. Finally, we address the issue of the band width of the HOMO state of C_{60}. We assert that the width of the photoemission peak of C_{60} does not reflect the intrinsic band width because it is broadened by the non 0–0 transitions via the Franck–Condon principle. Our view point provides a possible reconciliation between these photoemission data and those measured by other techniques.

1. Introduction

Buckminsterfullerene, a newly discovered form of pure carbon, is a molecule with 60 carbon atoms that occupy the 60 vertices formed by the intersections of 20 hexagonal and 12 pentagonal faces to form a hollow cage, as depicted in fig. 1. Due to the beauty of its highly symmetric structure, C_{60} has attracted much attention.

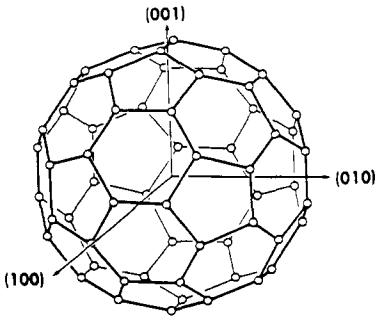

Fig. 1. Illustration of C_{60} molecular structure.

Theoretical conjectures of C_{60} clusters date back twenty years [1,2], and fullerene C_{60} was first identified in carbon vapor produced by laser irradiation of graphite in 1985 [3]. It was not until very recently that large quantities of C_{60} became available, which made it possible to discover the high-temperature superconductivity in alkali doped C_{60} [4–6], and to observe the large non-linear optical response [7]. These and other interesting properties of C_{60} stimulated research activities over the past two years [8]. By now, much effort has been made to carry out various experiments that reveal the geometric structure [9,10], the transport characteristics [11], and electronic structure [12–16], among other properties of this novel form of carbon. Theoretical calculations predict that C_{60} is a semiconductor with a direct gap of 1.5 eV [17].

Unlike graphite and diamond, solid C_{60} is a molecular crystal. The C–C bonds within an individual