06.3—9 EXPERIMENTAL AND THEORETICAL ANALYSIS OF THE INTERIONIC INTERACTIONS IN CRYSTALLINE LiCH. By E. Heuser-Hofmann and W. Weyrich, Faculty of Chemistry, University of Konstanz, Konstanz, Fed. Rep. of Germany.

In order to study the electronic structure of the covalent bond in CH , we have recently determined the complete three-dimensional electron momentum density and its Fourier transform (reciprocal form factor) in single-crystal LiOH using Compton scattering of 241-Am gamma-radiation. Apart from the strong anisotropy arising from the covalent bond in CH , the data show the influence of the interionic interactions in the crystal.

For the interpretation of these features we have applied Löwdin's symmetrical orthogonalisation method to freeion wave functions in clusters of varying size with the
appropriate spatial arrangement of the crystal structure. Approximations to Wannier functions have been obtained, from which we can analyse the nature of the
interionic interactions seen in the experimental data.

06.3-10 EXPERIMENTAL ELECTRON MOMENTUM DENSITIES IN TWO-DIMENSIONAL SOLIDS. By <u>G. Loupias</u> and J. Chomilier, Lab. de Cristallographie, U.P.M.C., ⁴ place Jussieu, 75230 Paris Cedex 05 and L.U.R.E., Bat 209C, 91405 Orsay Cedex, France.

The Compton profile is a very good experimental test for calculated wave functions because of its preferential sensitivity to valence and conduction electrons. The best resolution is obtained in the X-Ray range with a crystal analysis of the scattered photons: the Lure-DCI high resolution spectrometer was used for this study (Loupias et al. Phys. Stat. Sol. b 102, 79 (1980)). The insensitivity of this method to crystal defects makes it particularly suitable to understand the electron behaviour in graphite intercalation compounds. The first stage alkali compound is a sequence of successive alkali and carbon layers. The crystallites are randomly oriented in the basal plane but oriented along the \vec{c} axis.

The simplest model for LiC6, the rigid-band model, assumes that the Li 2s electron is totally transferred to a graphite Π band. A recent pseudo-potential calculation taking into account the valence band distorsion has been performed by Holzwarth and a Compton profile has been derived.

The Compton profiles have been measured with the same orientation of the scattering vector, for LiC6 and graphite. The experimental difference profile allows us to conclude about the electron behaviour: its excellent agreement with the last theory shows that it is necessary to consider both the charge transfer and the modification of the valence band in a so-called "Two dimensional" solid.

06.3-11 OFF-DIAGONAL MOMENTUM DENSITY OF SiBY MEANS OF COHERENT COMPTON SCATTERING. By W.Schülke, S.Mourikis, Institut für Physik, Universität Dortmund, D-4600 Dortmund 50, Fed.Rep. of Germany

As first pointed out by one of the authors (W.S, Phys.Lett.1981,83A,451) the measurement of the double differential cross section for inelastic X-ray scattering, where the initial photon state is the coherent superimposition of two plane waves in the Bragg case of diffraction, provides information about off-diagonal elements of the one particle density matrix in momentum space. This information can be obtained in the form of a one dimensional projection of the off-diagonal elements on the scattering vector (so called correlation profiles), where there exist certain intrinsic limitations with respect to the momentum resolution of this information. These limitations are discussed.

Then a method is presented, which utilizes information about the X-ray structure factor and the dynamical theory of X-ray diffraction in order to seperate correlation profiles from Compton profiles, which both appear superimposed in the measured double differential scattering cross section (DDSCS). By this means experimental correlation profiles of Si-valence electrons have been obtained by measuring DDSCS's at different positions of the Si-crystal within the Bragg reflection range utilizing a double crystal setting with a highly asymmetric cut first crystal. The solid state information made available by these measurements is outlined.

06.3—12 MOMENTUM SPACE ELECTRON DENSITY OF Li FROM DIRECTIONAL COMPTON PROFILES. By W. Schülke, T. Langer, P. Lanzki, Institut für Physik, Universität Dortmund, D-4600 Dortmund 50, Fed. Rep. of Germany.

With a momentum space resolution of 0.12 a.u. 10 directional Compton profiles (DCP's) of Li have been measured by means of a focusing crystal spectrometer with MoK -radiation utilizing a linear position sensitive detector. Effectively 5.10° counts have been accumulated in one profile. By using Fourier transform (FT) methods (Schülke, Phys.Stat.Sol.(b)1977,82,229; Hansen et.al.,Z.Phys.1982,B22,675) the three-dimensional momentum space electron density n(p) as well as the three dimensional occupation number density n(k) of Bloch states have been reconstructed from the DCP's. The reconstructed n(p) reveals well separated higher momentum components (HMC's) near the N-point of the Brillouin zone, whose amount could be fitted to Fourier components of the Li-pseudopotential. The reconstructed n(k) makes possible an estimate of electron correlation effects well separated from the influence of HMC's. Supported by model calculation the Fermi surface anisotropy of Li has been deduced from the FT of DCP's to be

$$(k_{[110]}^{F}-k_{[100]}^{F})/\bar{k}^{F}=(1.7\pm0.3)\cdot10^{-2}.$$

This is in good agreement with recent positron annihilation data.