

06.2-28 COMPARATIVE THEORETICAL STUDIES OF CHARGE DENSITY DISTRIBUTION IN GaAs, GaP, InAs AND InSb. By F. Meloni, Istituto di Fisica and GNSM-CNR, Università di Cagliari, Cagliari, Italy; M. Serra, Istituto di Astronomia e Fisica Superiore and GNSM-CNR, Università di Cagliari, Cagliari, Italy and A. Shaukat, International Centre for Theoretical Physics, Trieste, Italy and Physics Department, Punjab University, New Campus, Lahore-20, Pakistan.

Theoretical charge density distribution in four III-V semiconducting compounds has been calculated using various pseudopotential models. Whereas EPM calculations have been carried out following Cohen and Bergstresser (Phys. Rev. 141(1966), 789), use of soft-core (Appelbaum and Hamann, Phys. Rev. B(1975)) and hard-core model potential (Bertoncini and Meloni, J.Phys. C:Sol.State.Phys.(1984)) has been made for the self-consistent calculations of the charge density maps (110-plane) for different compounds. The analytic hard-core model potential can be written in real space as (in Å)

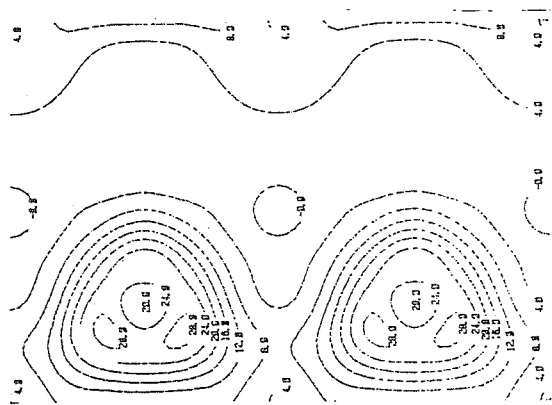
$$V(r) = \frac{-2Z}{r} (1 - e^{-\alpha r}) - B e^{-\beta r} + A r e^{-\alpha r}$$

where Z = no. of valence electrons; B and β are obtained by inverting the HF equation in the region at distance of nucleus; α is of the order of core radius and A is the resulting free parameter which reproduces the fundamental and excited electronic states and the s valence and p maxima of the HF wavefunctions in the nodeless regions. The parameters for InAs, for example, are

	A	α	B	β
In	134	3.4	21	3.0
As	530	5.0	29	4.6

All values are in atomic units. The model has shown its capability in solid state applications when applied to complex systems (Serra, Meloni and Baldereschi, Il Nuovo Cimento D2(1983), 1754). Comparison of the theoretical results can be made with the experimental charge density distribution studies for these compounds presented in this Congress (cf. Gomm).

Fig. 1 Valence charge density in InAs (hard model)



06.2-29 CHARGE DENSITY DISTRIBUTION IN SEMICONDUCTING COMPOUNDS OF THE III-V-TYPE. M. Gomm, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Loewenichstr. 22, Universität Erlangen-Nürnberg, FRG.

For the compounds GaP, GaAs, InAs and InSb experimental charge density distributions on the base of measurements already reported (M. Gomm, Acta Cryst. A34, S23) will be compared with theoretical calculations. A more sophisticated analysis of the original experimental data gave a remarkable improvement with respect to the R-values in the least squares procedures and in the valence and deformation Fourier syntheses. The discussion will be extended to measurements at room temperature.

06.2-30 ELECTRON DENSITY STUDY OF $\text{Co}(\text{C}_5\text{H}_5\text{NO})_6(\text{ClO}_4)_2$ AT 78K BY X-RAY AND NEUTRON DIFFRACTION. By J. S. Wood Chemistry Department, University of Massachusetts, U.S.A. and M. S. Lehmann and R. F. D. Stansfield, Institute Laue-Langevin, Grenoble, France.

The title complex is a member of the series of isostructural hexapyridine N-oxide complexes $\text{M}(\text{C}_5\text{H}_5\text{NO})_6\text{X}_2$ which at room temperature crystallise in space group $R\bar{3}$ with $Z = 1$. In addition to showing large trigonal electronic structural distortions, the complexes also exhibit interesting cooperative magnetic effects at low temperature which are dependent on the nature of the anion X, as well as the metal. In order to examine how these electronic properties are reflected in the charge density distribution around the metal and in the coordinated ligand, we have carried out low temperature X-ray and neutron diffraction measurements for the cobalt perchlorate complex. The X-ray data (10,994 measurements to $\sin \theta/\lambda = 1 \text{ \AA}^{-1}$ at 78K, 4,536 independent) have been used to calculate X-X(core) deformation density maps, while parameters obtained from the neutron refinement (1,359 independent reflections to $\sin \theta/\lambda = 0.67 \text{ \AA}^{-1}$ measured at 90K) have been used to calculate X-N maps. The neutron analysis shows the presence of a small amount of DMF solvent molecules coordinated to the metal, such that the composition of the crystal used for this analysis is actually $\text{Co}(\text{C}_5\text{H}_5\text{NO})_{5.7}(\text{DMF})_{.3}(\text{ClO}_4)_2$. Both sets of deformation maps show aspherical features around the cobalt atom attributable to the d-orbital density together with bonding and lone-pair features associated with the pyridine oxide ligand. The X-ray data are currently being analysed using multipole refinement methods and these results, together with a comparison with those reported for the free ligand, will be given.