

CONCLUSION

It has been demonstrated that analysis of the one-electron wave functions and energies calculated in the $X\alpha$ approximation can provide a basis for understanding a number of the physical properties of crystalline solids, including cohesion, p-V relationships, and phase transitions. X-ray spectra and magnetic properties have also been studied in the context of this approximation, to demonstrate their relationship to the energy-band properties of materials. The extension and refinement of studies of this general nature forms one aspect of the "perspectives for calculation of electronic properties in ordered and disordered solids".

ACKNOWLEDGEMENT

The authors are pleased to acknowledge the many stimulating and helpful conversations with members of the Quantum Theory Project about numerous aspects of the research reported herein.

One of them (J.B.C., Jr.) wishes to thank D. Nagel, R. Manne, E. Källne, E. Noreland, and L. Hedin for several very useful discussions regarding the measurement and interpretation of soft X-ray spectra, and K. Schwarz for much of the numerical data upon which the X-ray emission calculations are based. One of them (F.W.A.) is grateful for the cooperation of J. Springer and the Naval Weapons Laboratory for making possible several runs on their CDC 6700 computer. The major part of the computation was performed on the facilities provided by the University of Florida Computing Center.