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Symmetry and Bandstructure

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SYMMETRY AND BANDSTRUCTURE

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Received 17 December 1974

ADAPTATION SUMMARY

Title of adaptation: SYMMETRY AND BANDSTRUCTURE

Adaptation number: 0001

Reference to original program: Catalogue number: ACMJ;

Title: SYMMETRIZED APW; *Ref. in CPC:* 4 (1972) 361

Authors of original program: V. Hoffstein, D.K. Ray and M. Belakhovsky

Computer: Control Data CYBER 74

Operating system: SCOPE 3.4.1, level 373

Programming language used in adapted program: FORTRAN

High speed storage required: 70742 words

No. of bits in a word: 60

No. of cards required to effect adaptation: 39

Nature of physical problem

The program ACMJ (1) calculates the energy bands and electronic structure of cubic lattices with no more than two different atoms per unit cell.

Method of solution

The program was designed to run on an IBM computer and this adaptation converts it for use on CDC computers. The changes are also suitable for the program ACME [2].

The method of calculation of the bandstructure is the Symmetry Augmented Plane-Wave method (SAPW) which makes use of the point group symmetry of the hamiltonian.

Restrictions on the complexity of the problem

Only for cubic lattices.

Typical running time

For a 3×3 matrix eigenvalue problem calculated with ACMJ: 17 seconds with the LTN-compiler and 12 seconds with the RUN-compiler.

References

[1] V. Hoffstein, D.K. Ray, M. Belakhovsky, *Computer Phys. Commun.* 4 (1972) 361.

[2] V. Hoffstein and O. Moller, *Computer Phys. Commun.* 2 (1971) 17.

ERRATUM NOTICE

Title of manuscript: A general program to calculate the matrix of the spin-orbit interaction

Authors: W.-D. Klotz

Reference: Computer Physics Communications 9 (1975) 102.

Title of program: SPINORBITWEIGHTS

Catalogue number: AAKL

Title of manuscript: Program for spectra and cross-section calculations within the pre-equilibrium model of nuclear reactions

Author: E. Běták

Reference: Computer Phys. Commun. 9 (1975) 92.

Title of program: PREEQ

Catalogue number: ABGO