Polish J. Chem., **75**, 157–158 (2001) **BOOK REVIEW**

J. Mulak and Z. Gajek: **"The Effective Crystal Field Potential"**, Elsevier Science Inc., Amsterdam 2000.

At the first step, let me enjoy and welcome a scientific book written on a physical, or physico-chemical subject, by Polish authors. With the abundance of the literature devoted to humanistic subjects, met practically in any Polish so-called 'scientific' book-store, and an extremely scarce presence of real scientific literature met there, the book by Mulak and Gajek represents a nice exception and worth to be followed example.

The physical problem of the effective crystal field potential mentioned in the book title has been considered before by numerous approaches. For instance, we have an exhaustive treatment of the crystal core done by Harrison in his well-known book on the pseudo-potentials in metals; still other methods are connected with the quantum-defect approximation introduced to description of the crystal core and the band structure of the crystalline solids developed by Kuhn, Van Vleck and Ham. On the other hand, the subject of the modern book written by Mulak and Gajek is shifted evidently much more towards inorganic complexes and problems met in chemistry than towards the problems of a typical solid state.

The book begins on a rather advanced level which seems to be kept throughout a large part of the text. This aim seems to be ambitious, but – simultaneously – provides, in my opinion, an obstacle for an average physico-chemical reader. The first formula of the book, given on p. 1, is the effective Hamiltonian of the complex ion presented with the whole machinery characteristic for the spin-orbit coupling terms. But, simultaneously, no reference is given, or even mentioned, to this spin-orbit interaction effect; no physical description of the effect is given, neither are quoted the ideas being at the basis of the orbital angular momentum, or spin-angular momentum, operators. Moreover, the corresponding symbols entering the Hamiltonian remain fully unexplained. In total, this whole introductory formula makes an impression of a rather clever beginning, but certainly presents also, in its character, a little repulsive factor for an average chemical scientist.

The first chapters of the book are devoted to parametrization of the crystal-field Hamiltonian, also to a study of the effective crystal field potentials, as well as to construction of the wave functions, which describe an ionic complex or a quasi-molecular cluster. These problems refer certainly to the point-group symmetry species and notions, such as representations and the basis functions of representations characteristic for the applied point groups. Obviously, the group-theoretical notions and ideas are fundamental for the contemporary education of any quantum physicist, or theoretical chemist, nevertheless I feel that the gap between an average text-book level on the group theory and results, or ideas, presented on the same subject from the very beginning in the monograph prepared by Mulak and Gajek is too large. Numerous references, which are given by the authors to the corresponding literature, seem to be of not much help here, because most of them are also rather of a research level than represent digested studies having more explanatory properties. In total, in studying this group-theoretical part of the text, the reader misses the spirit of old, good reviews on the subject as those given in the book by Ballhausen (reference 38 of the Mulak-Gajek book) or in the didactically excellent article by Hutchings (reference 39), where careful explanations and numerous examples help evidently to understand better the scientific matter. It seems also to be a pity that authors, in their group-theoretical considerations, do not make any reference to the excellent review article on the group theory by Altmann and Cracknell [Revs. Mod. Phys., **37**, 19 (1965)]: the construction of the basis functions for the point-group symmetry species done from the spherical harmonics is presented there with a thoroughness, which seems to be difficult to surpass.

On the other hand, the presentation of the text concerning the density-functional theory and its applications to complex many-electron systems is done – in my opinion – in a much more accessible way. This concerns especially a brief survey of the local-density approximation, and the Kohn-Sham equations, accompanied by an outline of applications of these quantum-mechanical tools, especially to the case of the local spin-density effects. The concise sections devoted to the exchange-correlation problems, supplemented by a study of the self-interaction correction and the gradient approximation, seem to be also on a very good introductory level.

A nice surprise for a reader of the texts on the crystal field potentials is to find in the book a treatment of the electron screening effects, caused by the presence of the perturbations potentials, or defects, in the metallic materials. This kind of ideas is usually shifted to the text-books devoted to many-electron problems and theory of alloys and alloying. Here, we have a good sketch of presentation of the Fourier analysis of the screening, which is provided by a foreign potential acting on the electron charge distributed in a metal sample. This Fourier analysis is supplemented by the Thomas-Fermi calculation of the screened potential, screening radius and the static dielectric function, which are caused in the many-electron ensemble by a localized impurity. The plasmon effect of the screening of an external potential by the electron gas is also considered. The end of the Mulak-Gajek book gives a brief review of the effect done by the phonon dynamics on the static crystal-field picture and discusses the influence, which can be exerted on the crystal-field potential by the contributions obtained from a many-electron approach.

In total, I find the Mulak-Gajek text as well-written and interesting, although a little hermetic at its beginning part and, unfortunately, not without rather numerous printing errors contained in it. The book has been published by Elsevier in the Netherlands in the form of a rather nice volume. It is quite regrettable that such physico-mathematical publications seem to have at present no counterparts produced by the Polish editorial houses.

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