

# Vibronic Interactions: Jahn-Teller Effect in Crystals and Molecules

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# Vibronic Interactions: Jahn-Teller Effect in Crystals and Molecules

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**NATO Advanced Research  
Workshop  
on  
Colossal Magnetoresistance  
and Vibronic Interactions  
and  
The Fifteenth International  
Symposium on the  
Jahn –Teller Effect**

VIBRONIC INTERACTIONS IN CRYSTALS AND MOLECULES

*Boston*

The United States of America

**August 16 to August 22, 2000**

The host institutions are

**Boston University and Simmons College**

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## PREFACE

This book is based mostly on the reports presented at the XVth International Jahn-Teller Symposium on Vibronic Interactions in Crystals and Molecules and NATO Advanced Research Workshop Colossal Magnetoresistance and Vibronic Interactions that took place at Boston on August 16-22 of the year 2000.

This is the first time the Symposium took place in the USA where recently the giant splash of the attention to the Jahn-Teller effect occurred. This tremendous interest to the field all over the world is reflected not only in the numerous publications in many American and European Journals, but additionally in the Symposium's participation of the leading scientists from the well known Universities, National Laboratories and industrial companies, which was the largest in the history of the Symposium.

The renaissance of the Jahn-Teller physics is closely related to the three fundamental discoveries in science. The most significant among them is the discovery of high-Tc superconductivity by K.-A. Muller and G. Bednorz, for whom the "Jahn-Teller idea" was the motivation in their search. The result of this search is well known – a wide spectrum of the Jahn-Teller ion based materials with Tc between 24K and 135K were found. The second discovery is the existence of a new polymorph of carbon – the C<sub>60</sub>. The microscopic analysis of all physical, chemical and biological properties of the buckyballs is based on Jahn-Teller type of interactions. The third is colossal magnetoresistance. This phenomenon was recently rediscovered in the manganese oxide compounds and attracts attention not only for its very rich physics but also for its very promising applications in industry. And here once again the Jahn-Teller ion – ion with orbitally degenerate or pseudo degenerate electronic ground state – plays the major role in the most of the material properties.

Turning again to the particulars of the XVth Jahn-Teller Symposium, we would like to comment on one of its distinguishing features. For the first time, the father of the Jahn-Teller effect, Prof. Edward Teller participated in the Symposium. While his illness restricted him from coming to Boston and delivering his talk at the time of the Symposium, we were able to meet him in advance and to record his greeting and a presentation to the participants. His brief historical remarks, opinions on the role of the Jahn-Teller effect in Materials Science and high-Tc superconductivity, and some of his novel ideas will be of interest to the readers.

It is our hope that the book will be helpful to the scientists interested in colossal magnetoresistance, high-Tc superconductivity, buckyballs, and new magnetics with orbital degeneracy. Quite often, the new enthusiasm in one of the science fields is accompanied by "rediscoveries". This book should save some work time for those interested in the electron-phonon interaction at orbital degeneracy – the Jahn-Teller effect, - while, of course, it does not contain ready solutions to many of the problems.

One of the goals of the XVth Jahn-Teller Symposium was to bring together scientists from different fields – physics, chemistry, biology--, who are working on Jahn-Teller problems, for developing a “common language and common ideological platforms”. That is why in the Program of the Symposium the different subject presentations are next to each other.

The structure of the book corresponds in this sense to the structure of the Symposium. There are “short” (4-5 pages) and “long” (8-16 pages, related to the invited talks) manuscripts on different subjects. The reader will find in the book, for example, the results of the experimental studies and reviews on colossal magnetoresistance (J. Goodenough and Zhoo, D. Looca, C. Nelson), chemical point of view on high-Tc superconductivity (W. Grochala and R.Hoffmann) and materials science of perovskites (M. Atanasov and D. Reinen), vibronic interactions in biological systems (M. Belinski, S. Stavrov) and molecules (C. Bates, J. Dunn, M. Abou-Gantous), theoretical studies of colossal magnetoresistance (L. Gor’kov, V. Kresin, and M. Dzero) and structural phase transitions (M. Kaplan, B. Vekhter, G. Zimmerman), high-Tc superconductivity (A. Bratkovsky, V. Polinger, D. Haskel, A. Stern), fundamental questions of the Jahn-Teller effect (I. Bersuker, A. Ceulemans, Q. Qiu). However, all the manuscripts on the different subjects have a commonality, the Jahn-Teller, or vibronic, approach. This should be of interest to the reader from any of these fields.

Of course, it is difficult to convey the atmosphere of excitement and creative energy that pervaded the Symposium. As the participants are acknowledging, the Symposium and the NATO ARW were most successful. This was made possible by the support of the meeting’s sponsors. The financial support of NATO’s Science Division was crucial for the success of the Symposium. The organizational and financial help of the hosts of the meeting Boston University and Simmons College can not be overestimated. The support of MKS, Elsevier Publisher, and Mitre is gratefully acknowledged.

We would like to thank all authors for their contributions and time it took them for preparing the manuscripts.

Michael Kaplan,  
George Zimmerman.