
Preface

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This issue contains a selection of articles presented at the eleventh Brazilian Symposium on Theoretical Chemistry, held in Caxambu, MG, Brazil, 18–21 November, 2001.

The first Brazilian Symposium on Theoretical Chemistry (SBQT) took place in the city of Rio de Janeiro, on November 1981. Motivated by the eagerness of the scientific community that, although small at that time, felt the lack of interaction amongst the theoretical groups and experimentalists, in a country with continental dimension and until then with very poor means of communication. Since then the community decided to have a similar event every two years in different regions of the country. The symposium has been held, since the fourth SBQT, at the Hotel Gloria, Caxambu, State of Minas Gerais. Caxambu is in a convenient geographical place situated at approximately equal distance from the main southeast capital cities Rio de Janeiro, São Paulo and Belo Horizonte.

The SBQT was born with three main objectives: (i) to promote an interaction between theoreticians and experimentalists (ii) to publicize the work realized in the country (iii) to valorize the theoretical area as a whole. The symposium reached the eleventh edition, faithful to the original objectives, which were broadened over the last twenty years, with admirable and unquestionable success. Nowadays the SBQT constitute the biggest and most important theoretical scientific event in the Latin America, propitiating a rich and stimulating envi-

ronment for scientific discussion, being extremely motivating for students and young researchers.

The contribution of the SBQT to the development of the theoretical area in the country is undeniable. Theoretical chemistry, considered in the past as an area of purely academic interest, is now recognized of great importance in the formation of modern chemists. The graduate and post-graduate courses addressing theoretical chemistry has multiplied all over the country. In the present time the theoretical chemistry in Brazil encompass contributions from various specific areas such as Quantum Chemistry, Atomic and Molecular Dynamics, Computational Simulation of Liquid and Solid systems, Molecular Modeling of Systems of Biological and Technological interest, Chemical Catalysis, Physical Organic Chemistry among others. Although the SBQT has, beyond any doubt, contributed to the increase in the scientific production of the theoretical area, the most outstanding contribution is the enhancement of the quality of the scientific work produced in the country. In quantitative terms, from 53 contributions presented in the first SBQT (1981), we reached more than 400 in the XI-SBQT (2001).

In 2001, the SBQT is completing 20 years of existence, an outstanding achievement, a result of the joint efforts from the whole community keeping two decades of tradition in theoretical chemistry in the country. In this symposium, as it has been happening in previous years, the topics of the plenary talks will be the most diversified as possible, aiming to cover the distinct areas of research existent in the

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theoretical community of our country. The participants of the XI-SBQT came from different parts of the world, including South and Central America and also invited scientists from the USA and Europe. We thank all of them for contributing to make the XI-SBQT so scientifically profitable and pleasant. We are also grateful to the financial support from the Brazilian agencies CAPES, CNPq, FACEPE, FAPEMIG, FAPERGS, FAPERJ, FAPESP, FUNDEP, PRPq-UFMG.

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