

## Editorial

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# Special issue: IV Congress of Theoretical and Computational Physical Chemistry. 26–28 of November of 2012, Altos de Pipe, Caracas, Venezuela

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This special issue of the Journal of Computational Methods in Science and Engineering (JCMSE) consists of a selection of papers about the presentations in the IV Congress of Theoretical Physical and Computational Chemistry (IV-CFQTC), held at Altos de Pipe, Caracas, in the Instituto Venezolano de Investigaciones Científicas (IVIC), from 26 to 28 November 2012. The articles were written by the most important Venezuelan scientists in areas of molecular modeling, theoretical chemistry, computational catalysis, bioinformatic and medicinal chemistry, calculations of reaction mechanisms and kinetics, prediction of molecular electric and magnetic properties, and chemical process simulation in the industry.

Several international invited researchers attended to the IV-CFQTC with 9 plenary lectures of high scientific quality and 68 posters distributed into two sessions were also presented. The attendance was more than 100 participants from different universities and research institutes.

### **International Invited Speakers:**

**Albeiro Restrepo**

Universidad de Antioquia, Colombia.

**Alberto Vela**

CINVESTAV, México.

**Guillermo Restrepo Rubio**

Universidad de Pamplona, Colombia.

**João B.L. Martins**

Universidade de Brasilia, Brasil.

**Kleber C. Mundim**

Universidade de Brasilia, Brasil

**Luis Javier Álvarez**

Universidad Autónoma de México.

**Lucyna Firlej**

Université de Montpellier, France.

**Mathias Rapacioli**

Université Paul Sabatier, France.

**Roberto Gomperts**

NVIDIA Corporation, USA

In addition, 16 short talks were presented by different research groups in Venezuela.

Participants were invited to submit manuscripts of their presentation for a JCMSE special issue, and 18 of them were accepted after a careful peer review process. We wish to thank the speakers for their splendid and interesting conferences. Also, we greatly appreciate all the persons and institutions allowing the IV-CFQTC to be organized in Venezuela: INTEVEP-PDVSA, Academia Venezolana de Ciencias Físicas Matemáticas y Naturales, FONACIT, IVIC, Red Venezolana de Nanotecnología, and also private enterprises as Fundación Empresas Polar. They kindly contributed to the costs of travelling and lodging of some of the invited speakers. The offer of the JCMSE to publish extended papers, after peer review, is gratefully acknowledged.

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