

Editorial

Special issue: II Congress of Theoretical and Computational Physical Chemistry. 2–4 of December of 2008, Choroní, Venezuela

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The present issue of the Journal of Computational Methods in Science and Engineering (JCMSE) is especially devoted to the II Congreso de Físicoquímica Teórica y Computacional (II Congress of Theoretical and Computational Physical-Chemistry) (II CFQTC). This Congress took place at Choroní, Venezuela, December 2–4 of 2008.

II CFQTC has considered different areas of general interest: molecular modeling, theoretical chemistry, computational catalysis, bioinformatic and medicinal chemistry, calculations of reaction mechanisms and kinetics, prediction of molecular electric and magnetic properties and finally and chemical process simulation in the industry.

Invited researchers attended to the Congress (8 plenary lectures), all of them, of high scientific quality, as confirmed by their recent publications and curriculum vitae. Moreover, more than 80 posters distributed into three sessions were also presented. The subjects and corresponding invited opening lectures were:

1. Predictive QSAR modeling and virtual screening: Alexander Tropsha (USA).
2. Cálculos ab-initio de estructuras electrónicas con cota de error: Carlos Bunge (Mexico)
3. VEGA ZZ: a versatile toolkit for drug design and protein modeling: Alessandro Pedretti (Italy)
4. Theoretical calculations associated with high vibrational levels: spectroscopy and kinetics: Carlos Manzanares (USA)
5. Tres técnicas nuevas en la teoría de ab initio del propagador del electrón: Vincent Ortiz (USA)
6. Desulfuración sobre carburos y sulfuros metálicos: papel de los átomos C y P: Jose Antonio Rodríguez (USA)
7. CNTQ: Vinculación Universidad – sector productivo: Humberto Soscún (Venezuela)

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8. Radiative and Auger data for modeling Ni K lines: Patrick Palmeri (Belgium)

The attendance was circa 100 participants coming from different universities and researches institutes. All participants were encouraged to submit manuscripts of their presentation for a JCMSE special issue, from which 16 of them were accepted after a careful peer review process. We wish to thank the speakers for their lucid and interesting conferences. Also, we greatly appreciate all the persons and institutions allowing II CFQTC to be held in Venezuela: Instituto Venezolano de Investigaciones Cientificas (IVIC), Intevep - PDVSA, Centro Nacional de Tecnología Química (CNTQ), Universidad Simón Bolívar (USB), Universidad Central de Venezuela (UCV) and La Universidad del Zulia (LUZ) and also private enterprises as Fundación Polar. They kindly contributed to the costs of travelling and lodging of some of the invited speakers. We would like to make a special mention to all the referees that contributed with the reviewing of the manuscripts for this issue and Lic. Vanessa Duarte (CNTQ) who helped the Guest Editors to prepare this special issue. Their collaboration made possible the present publication. Finally, and also important, we would like to express our warmest gratitude to all participants to the Congress, because they truly played an important role in the success of this event.