Aims & Scope
The major goal of the JCMSE is the publication of new research results on computational methods in sciences and engineering. Common experience had taught us that computational methods originally developed in a given basic science, e.g. physics, can be of paramount importance to other neighbouring sciences, e.g. chemistry, as well as to engineering or technology and, in turn, to society as a whole. This undoubtedly beneficial practice of interdisciplinary interactions will be continuously and systematically encouraged by the JCMSE. Moreover, the JCMSE shall try to simultaneously stimulate similar initiatives, within the realm of computational methods, for knowledge transfer from engineering to applied as well as to basic sciences and beyond.

This special issue brings together contributions by eminent specialists in the field of the theoretical determination of electric polarizability. The contents of the issue cover a wide area of subjects relevant to Chemical Physics, Molecular Physics, Nonlinear Optics and Materials Science.

Specific subjects
Ab initio and Density functional theory calculations of electric polarizability and hyperpolarizability, intermolecular forces, aromaticity, molecular design, electric properties of solvated molecules, NLO materials, Raman intensities, polarizability of metal and semiconductor clusters, relativistic effects on electric properties, and more.

Special Issue: Computational aspects of electric polarizability calculations: Atoms, molecules and clusters

Guest Editor: Professor George Maroulis, Department of Chemistry, University of Patras, Greece

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- Dipole polarizability and second hyperpolarizability of difluoroacetylene: basis set dependence and electron correlation effects/ M. Medved, B. Champagne, J. Noga and E.A. Perpète
- PLS prediction of hyperpolarizabilities for donor-bridge-acceptor organic systems/ A.E. de A. Machado, B. de Barros Neto, A.A. de S. da Gam
- Collisional polarizability correlation functions. A step towards rotational-translational coupling/ W.Glaz
- Density functional calculations of the frequency-dependent optical rotation: comparison of theory and experiment for the gas phase/ C. Diedrich, S. Kaasemann and S. Grimme
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• First hyperpolarizability of 6-vertex carboranes 2. DFT study of NH3/N2O2-substituted 1,2-closo-dicarbahexaboranes/ K. Yu Suponitsky and T.V. Timofeeva
• Polarizabilities of amino acid residues/ M. Swart, J.G. Snijders and P.Th. van Duijnen
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