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GUEST EDITORIAL

Guest editorial

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The present issue of the Journal of Mathematical Chemistry collects selected articles on topics addressed at the International Conferences on Mathematical Methods for Ab Initio Quantum Chemistry, held at the University of Nice-Sophia Antipolis between 2006 and 2010. It is a follow up to the special issue for the 2005 conference.

These meetings are designed to give the opportunity to mathematicians and theoretical chemists to discuss topics of common interest and cross-fertilize their approaches.

The topics found in this issue include reduced density matrices and geminal functions as alternative to describe electron correlation in molecular systems; Hopf algebra techniques to deal with the combinatorics occurring in matrix element calculations as well as in diagrammatic approaches to perturbative expansions; the derivations and applications of potential energy surfaces in molecular spectroscopy and dynamics; new developments in infra-red and microwave computational spectroscopy and their applications to biological systems, atmospheric sciences and astrochemistry.

We hope that this special issue will contribute to tighten the bonds between the mathematics and chemistry communities, just as the conferences do.

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