Editors:
Prof. Ray Hefferlin, Southern Adventist University, TN, USA
Prof. Maurice R. Kibler, Université de Lyon, France

COMPUTATIONAL CHEMISTRY and APPLICATIONS in ELECTRONICS

Published by WSEAS Press
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Proceedings of the 1st WSEAS International Conference on COMPUTATIONAL CHEMISTRY (COMPUCHEM '07)

Mathematics and Computers in Science and Engineering
A Series of Reference Books and Textbooks

Cairo, Egypt, December 29-31, 2007

ISBN: 978-960-6766-26-8
ISSN: 1790-2769

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Preface

The book you are currently holding contains the proceedings of the 1st WSEAS International Conference on Computational Chemistry (COMPUCHEM'07) which was held in Cairo, Egypt, December 29-31, 2007

The WSEAS conference COMPUCHEM is a new conference of the society and attracted very good contributions in Computational Chemistry as well as various applications in Chemical Engineering and Electronics. We hope with your help to increase the size of the conference in the next years and make it large as the other high-quality WSEAS events.
The COMPUCHEM aims to disseminate the latest research and applications in the afore mentioned fields. The friendliness and openness of the WSEAS conferences, adds to their ability to grow by constantly attracting young researchers. The WSEAS Conferences (in general) attract a large number of well-established and leading researchers in various areas of Science and Engineering as you can see from http://www.wseas.org/reports . Your feedback encourages the society to go ahead http://www.worldses.org/feedback.htm
The WSEAS meetings have always a special appeal to young researchers and are characterized by a friendly atmosphere in which delegates at different stages of their careers can talk to each other.

We would like to address to each of you a warm invitation for the 7th WSEAS International Conference on ARTIFICIAL INTELLIGENCE, KNOWLEDGE ENGINEERING and DATA BASES (AIKED'08) (that will be held in the University of Cambridge) where our "father" Prof. **Lotfi A. Zadeh** will be for 4th time Plenary Speaker in a WSEAS Congress presenting the Plenary Lecture: *"Toward Human-Level Machine Intelligence"*. Details:
http://www.wseas.org/conferences/2008/cambridge/aiked/Plenary1.htm

The contents of this Book are also published in the CD-ROM Proceedings of the Conference. Both will be sent to the WSEAS collaborating indices after the conference: www.worldses.org/indexes.

In addition, papers of this book are permanently available to all the scientific community via the WSEAS E-Library.

Expanded and enhanced versions of papers published in these conference proceedings are also going to be considered for possible publication in one of the WSEAS journals that participate in the major International Scientific Indices (Elsevier, Scopus, EI, Compendex, INSPEC, CSA .... see: www.worldses.org/indexes) these papers must be of high-quality (break-through work) and a new round of a very strict review will follow. (No additional fee will be required for the publication of the extended version in a journal).

We cordially thank all the people of WSEAS for their efforts to maintain the high scientific level of conferences, proceedings and journals.

The Editors

Plenary Lecture I

Through the Element Chart into Periodic Systems of Molecules

Prof. Ray Hefferlin
Southern Adventist University
TN, USA
hefferln@southern.edu

Abstract: Imagine that one of the compartments of the element chart is a door through which we can enter to explore molecular space. Suppose that the door we select is labelled "C". We enter and find all diatomic molecules with a carbon atom. After repeating this brief exploration for all the doors, we find that to a very good approximation, the properties of free diatomic molecules echo analogous properties (e.g., "sizes," high-energy cross-sections) of the two atoms which form them. We can express this mathematically by embedding the element chart in a null matrix and taking the outer product of the matrix with itself. This elegant four-dimensional system covers several proposed periodic charts of diatomic molecules: their originating element charts can be subjected to outer multiplication in silico to reproduce them. Graph-plotting and least-squares smoothing applications were used extensively with show the faithfulness of the four-dimensional periodic system of diatomic molecules. It has been used to forecast data (using neural-network protocols) such as 1,920 new ground-state vibration frequencies. The average 1% confidence limit is 10.66%; the accuracy is such that the forecasts for 221 of 224 training molecules agree with the training data within the forecasting confidence limits or fall outside by less than 10% of the training values, and 181 agree within the confidence limits. Returning to our starting point, we can re-enter the doors and go farther to explore all triatomic molecules with one or more carbon atoms. Data for gas-phase triatomics also manifest periodicity, and we can take the outer product of the element-chart matrix with itself twice to form the periodic system of triatomic molecules. Such systems also have been used in the predictive mode with the help of multiple-regression and neural-network executables. Yet again we can re-enter and explore classes of larger species (e.g., halomethanes) in various phases; again we use graphics applications and we discover periodicity and second periodicity sufficiently-well resolved that we can forecast data for numerous properties. Finally, we can enter still once more and explore species, whatever their atomic constituents, that have the same total electron number as the element whose door we select. This entry allows the study of ionized and quarked molecules, and the linking of all periodic systems by means of hyper-periodicity.

Brief Biography of the Speaker: Dr. Ray Hefferlin was born in Paris, France, and went with his father to the United States because World War II was imminent. His education took place at the University of California, Berkeley, at Pacific Union College (BA, physics), and at the California Institute of Technology (PhD, Physics). He has been a member of the faculty of Southern Adventist University since 1955. Dr. Hefferlin took leaves of absence at universities in Tennessee, Colorado, and Leningrad. He consulted at the National Institute of Science and Technology (spectral-feature intensity constants) and at laboratories of the DOE

(spectroscopic studies of rare-gas quenching and impurity species in thermonuclear fusion reactors) and NASA (optical spectroscopic studies of the luminous plumes resulting from entry of spacecraft into the atmospheres of the earth and other planets). This laboratory work stimulated the interest in periodic systems of molecules, a field to which he with his students and colleagues world-wide have contributed some 50 publications. Dr. Hefferlin's wife, Inelda, is from California. She is very active in civic affairs. They enjoy travelling, languages, and hiking. Their family includes four daughters and sons-in-law, and six grandsons.

Plenary Lecture II

Bases in Quantum Chemistry, Quantum Computation And Quantum Information

Prof. Maurice R. Kibler
Université de Lyon,
Institut de Physique Nucléaire,
université Lyon 1 and CNRS / IN2P3,
43 Bd du 11 Novembre 1918,
F-69622 Villeurbanne Cedex, France
m.kibler@ipnl.in2p3.fr

Abstract: The interest of symmetry adapted bases (atomic orbitals, molecular orbitals, spin waves, etc.) is well-known in quantum chemistry. In particular, the spherical harmonics (e.g., in atomic spectroscopy) and cubical, tetragonal or trigonal harmonics (e.g., in crystal-field theory and ligand field theory) is quite familiar to the practitioner in theoretical chemistry and chemical physics. The symmetry adapted functions generally span bases for finite-dimensional Hilbert spaces associated with reducible or irreducible representations of a symmetry group. A Hilbert space of finite dimension d can describe a system of qudits (qubits correspond to d=2, qudits to d arbitrary) used in quantum computation and quantum information. It is the object of this paper to construct bases which play an important role in quantum measurements and quantum information theory (quantum state tomography and quantum cryptography). Such bases, as for example mutually unbiased bases (MUBs) and positive operator valued measures (POVMs) bases, can be generated from methods similar to the ones used for building symmetry adapted bases. We develop here an approach that gives a complete solution for the construction of MUBs in the case where the dimension d of the considered Hilbert space is a prime number. We also give the starting point for studying the case where d is the power of a prime number.

Brief Biography of the Speaker:

Professor Maurice R. Kibler is a theoretician interested in applications of quantum mechanics and group theory to theoretical physics, mathematical physics and quantum chemistry. Symmetries and supersymmetries, based on the use of groups (finite groups, Lie groups, graded Lie groups, and quantum groups) as well as algebras (Lie algebras, graded Lie algebras, Hopf algebras, and quantum algebras), play a central role in his researches achieved alone or in the framework of numerous collaborations. These researches can be classified into several categories. (1) In crystal- and ligand-field theory, he established a connection between the point charge electrostatic model and the angular overlap model. Furthermore, he developed a model, through the use of the Wigner-Racah algebra of a chain of groups starting with the group SU(2), for describing the energy levels and the intensities of multiphoton electronic transitions for a partly-filled shell ion (transition metal or lanthanide or actinide ion) in a surrounding with a given symmetry. (2) He contributed to the development of invariance and noninvariance dynamical groups and quantum groups for dynamical systems in: (i) atomic spectroscopy (in connection with the SO(4,2) symmetry of the hydrogen atom, the Hartmann system of quantum chemistry and related systems, a deformed Aufbau Prinzip, and the periodic table of chemical elements); (ii) in molecular and nuclear physics (for the study of vibrational and rotational bands of molecules and deformed and superdeformed nuclei); and (iii) in particle physics (for the study of quantum-deformed dual amplitudes). (3) He also introduced the concept of k-fermions, which are objects interpolating between fermions and bosons, and contributed, via the introduction of a generalized Weyl-Heisenberg algebra, to the development of fractional supersymmetric quantum mechanics. (4) In

mathematical physics, he made important contributions to the study of the Wigner-Racah algebra of a chain of finite or compact groups, he developed the notion of nonbijective canonical transformations (in connection with Cayley-Dickson algebras and Hopf algebras), and he introduced the concept of Lie algebras under constraints. (5) Most of his present researches are devoted to fractional supersymmetric quantum mechanics (with the study of shape invariant potentials) and to quantum information theory (with the study of bases useful in quantum information and quantum computation). In particular, he is involved in the understanding of the so-called mutually unbiased bases (used in quantum cryptography and quantum tomography) and positive operator valued measures (used in quantum measurements).

Prof. Kibler is a member of the Theory Group of the Institute of Nuclear Physics of Lyon (a component of the IN2P3/CNRS, France). He teaches mathematics for physicists and engineers at the University Lyon 1 (a component of the University of Lyon) and at the ARCNAM Rhone-Alpes (a component of the CNAM, France). He is the author or co-author of 160 scientific publications in journals, books and proceedings, of several articles in encyclopedias, and of one textbook. He is regularly involved in international conferences and workshops.

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