INTRODUCTION

The quantum world of molecules: from orbitals to spin networks

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The advent of quantum mechanics, at the beginning of the Twentieth Century, revolutionized the way to describe and interpret nature at the molecular level. The thirty years of the short happy life of chemistry as a science passed through the interpretation of electromagnetic radiation emitted by a black body (M. Planck) and the introduction of the concept of light quanta (A. Einstein), the orbital angular momentum quantization (N. Bohr and A. Sommerfeld), the formulation of a wave equation for atomic orbitals (E. Schrödinger), the spin angular momentum (W. Pauli and P. Dirac), until the famous Dirac's statement: "The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved", that appeared to ratify the end of chemistry as a basic science, only confined to the task of numerical solutions for perhaps impervious equations. All of them were Nobel laureate in Physics, nevertheless chemists know well for example how the above story was influenced not only by the periodic system but also by the evidence that the covalent bond is due to couplings of electrons through their magnetic moments (G. N. Lewis). Well established along all the following decades, and worth of being documented regarding current research, is that impressive progress is coming not only

by increased computational power, but also by ingenious advances, as pioneered by Linus Pauling and many other quantum chemists.

In this issue and in the next one, a special section is dedicated to the International Conference "The quantum world of molecules: from orbitals to spin networks" held at the Accademia dei Lincei in Rome, 27–28 April 2017. It was organized by the Academicians Vincenzo Aquilanti (chairman, Perugia), Vincenzo Barone (Pisa), Sergio Carrà (Milan), Dante Gatteschi (Florence), Vincenzo Schettino (Florence), Antonio Sgamellotti (Perugia) and Giuseppe Zerbi (Milan), and by Federico Palazzetti from the Università di Perugia. The event was supported by the Fondazione Guido Donegani and with the collaboration of the Accademia Nazionale delle Scienze o dei XL and the Dipartimento di Chimica, Biologia e Biotecnologie of the Università di Perugia. The conference was dedicated to the commemoration of three influential Academicians: Massimo Simonetta (1920–1986), Eolo Scrocco (1926–2012) and Gian Gualberto Volpi (1928–2017), who greatly contributed to experimental physical chemistry. This conference has the same format of those dedicated to the Astrochemistry (Lincei 2011) and Chirality (Lincei 2013), recorded in dedicated issues of Rendiconti Lincei, as a series of general talks accounting for recent progress and also of presentations of current research results.

The discussion involved the following topics: (1) quantum chemistry applied to electronic structure and dynamics calculations; (2) molecular magnetism and application of spin-based properties; (3) the state-of-art of experimental techniques and theoretical tools for the study of reaction dynamics, including the development of methods of molecular orientation and the characterization of molecular interactions; (4) the manifestation of chirality from a physico-chemical point-of view; (5) spin networks.

The talks of the conference, introduced by Maurizio Brunori, president of the Fondazione Donegani and

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Vincenzo Aquilanti, were the following: “Spintronic and chirality” (Ron Naaman, Weizmann Institute of Science, Rehovot); “Space–time distribution of reaction products” (Piergiorgio Casavecchia, Università di Perugia); “Stereodynamical role of orbital spatial orientation in chemical reactions” (Toshio Kasai, Osaka University); “Vectorial imaging of photoprocesses” (King-Chuen Lin, National Taiwan University, Taipei); “Magnetic molecules at the interface: hybrid architectures for spintronics” (Matteo Mannini, Università di Firenze); “Molecular magnetism: a promising route towards a quantum computer” (Stefano Carretta, Università di Parma); “Anisotropic forces and molecular dynamics” (Fernando Pirani, Università di Perugia); “The astrochemical observatory and the search for chirality” (Andrea Lombardi and Federico Palazzetti, Università di Perugia); “Semiclassical mechanics of Wigner–Racah coefficients” (Robert Littlejohn, University of California, Berkeley); “Spin networks as combinatorial space-times” (Annalisa Marzuoli, Università di Pavia); “True chiral effects in the presence of magnetic fields” (Paolo Lazzeretti, Università di Modena e Reggio Emilia); “Angular momentum states, non-Euclidean extensions and applications” (Roger Anderson, University of California, Santa Cruz); “Vector correlation and polarization in photofragmenting molecules” (Oleg Vasyutinskii, IOFFE Institute, St. Petersburg); “Basis sets and their convergence properties” (Antonio Varandas, Universidade de Coimbra); “Spin states of the light atoms” (M. Belen Ruiz, Friedrich-Alexander-University of Erlangen-Nürnberg); “Relativistic quantum chemistry involving heavy atoms” (Leonardo

Belpassi, ISTM-CNR, Perugia—Francesco Tarantelli, Università di Perugia); “Wave equations on discrete non-Euclidean surfaces” (John Avery and James Avery, University of Copenhagen); “Kepler–Coulomb orbitals and orthogonal complete polynomial sets” (Cecilia Coletti, Università G. D’Annunzio Chieti-Pescara); “Slater-type orbitals in molecular electronic structure calculations” (Philip Hoggan, Institut Pascal, Clermont-Ferrand—Ali Bagci, University of Warsaw); “Spectroscopic accuracy: the role of electron correlation and basis set” (Cristina Puzzarini, Università di Bologna); “Montecarlo orbitals of confined atoms” (Savino Longo, Università di Bari); “Non-adiabatic Ring-Polymer molecular dynamics” (Danilo Calderini, ETH Zurich); “Discretized harmonics for large angular momentum reactivity” (Dario De Fazio, ISM-CNR, Rome); “Chemical dynamics through propagation of localized orbitals” (Dimitrios Skouteris, Scuola Normale Superiore di Pisa). Chairmen of the sessions were Sergio Carrà, Roberta Sessoli (Università di Firenze), Vincenzo Schettino, Sergio Abbate (Università di Brescia), Vincenzo Barone, Antonio Sgamellotti.

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References

- Rend. Fis. Acc. Lincei (2011) 22:67–172, 173–224, 375–394
- Rend. Fis. Acc. Lincei (2013) 24:177–308