ACCADEMIA NAZIONALE DEI LINCEI

FONDAZIONE «GUIDO DONEGANI»

INTERNATIONAL CONFERENCE

THE QUANTUM WORLD OF MOLECULES: FROM ORBITALS TO SPIN NETWORKS

April 27 - 28, 2017

Organizing committee: Vincenzo AQUILANTI (Chair), Vincenzo BARONE, Sergio CARRÀ, Dante GATTESCHI, Federico PALAZZETTI, Vincenzo SCHETTINO, Antonio SGAMELLOTTI, Giuseppe ZERBI

Ninety years ago a scientific revolution, the advent of quantum mechanics, provided conceptual and practical ingredients for describing and controlling nature at the molecular level: a survey is proposed of the state-of-the-art and of perspectives. Topics are selected in view of their basic experimental and theoretical relevance in modern molecular sciences and in quantum chemistry. The three-half-days structure of the conference follows the previous events on Astrochemistry (2011) and Chirality (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.

PROGRAMME

Thursday, 27 April

The modern experimental perspective

14.00 Welcome address by Maurizio BRUNORI (Presidente della Fondazione Donegani)

14.10 Vincenzo AQUILANTI (Linceo, Università di Perugia): Introduction

Chair: Sergio CARRÀ (Linceo, Politecnico di Milano)

14.30 Ron NAAMAN (Weizmann Institute of Science, Rehovot): *Spintronic and chirality*

15.05 Piergiorgio CASAVECCHIA (Università di Perugia): *Space-time distribution of reaction products*

15.30 Toshio KASAI (Osaka University): *Stereodynamical role of orbital spatial orientation in chemical reactions*

15.55 King-Chuen LIN (National Taiwan University, Taipei): *Vectorial imaging of photoprocesses*

16.20 Coffee break

Chair: Roberta SESSOLI (Università di Firenze)

16.40 Matteo MANNINI (Università di Firenze): *Magnetic molecules at the interface: hybrid architectures for spintronics*

17.00 Stefano CARRETTA (Università di Parma): *Molecular magnetism: a promising route towards a quantum computer*

17.20 Fernando PIRANI (Università di Perugia): *Anisotropic forces and molecular dynamics*

17.45 Andrea LOMBARDI, Federico PALAZZETTI (Università di Perugia): *The astrochemical observatory and the search for chirality*

Friday, 28 April

Spin networks and molecular orbitals

Chair: Vincenzo SCHETTINO (Linceo, Università di Firenze)

9.30 Robert LITTLEJOHN (University of California, Berkeley): *Semiclassical mechanics of Wigner-Racah coefficients*

10.00 Annalisa MARZUOLI (Università di Pavia): *Spin networks as combinatorial space-times*

10.25 Paolo LAZZERETTI (Università di Modena e Reggio Emilia, Modena): *True chiral effects in the presence of magnetic fields*

10.50 Roger ANDERSON (University of California, Santa Cruz): *Angular momentum states, non-Euclidean extensions and applications*

11.15 Coffee break

Chair: Sergio ABATE (Università di Brescia)

11.30 Oleg VASYUTINSKII (Ioffe Institute, Saint Petersburg): *Vector correlation and polarization in photofragmenting molecules*

11.55 Antonio VARANDAS (Universidade de Coimbra): *Basis sets and their convergence properties*

12.20 M. Belén RUIZ (Friedrich-Alexander-University of Erlangen-Nürnberg): *Spin states of the light atoms*

12.45 Leonardo BELPASSI (ISTM-CNR, Perugia) – Francesco TARANTELLI (Università di Perugia): *Relativistic quantum chemistry involving heavy atoms*

Chair: Vincenzo BARONE (Linceo, Scuola Normale Superiore, Pisa)

14.00 John AVERY, James AVERY (Københavns Universitet): *Wave equations on discrete non-Euclidean surfaces*

14.25 Cecilia COLETTI (Università G. D'Annunzio, Chieti): *Kepler-Coulomb orbitals and orthogonal complete polynomial sets*

14.50 Philip HOGGAN (Institut Pascal, Clermont-Ferrand) - Ali BAGCI (Uniwersytet Warszawski): *Slater-type orbitals in molecular electronic structure calculations*

15.15 Cristina PUZZARINI (Università di Bologna): *Spectroscopic accuracy: the role of electron correlation and basis sets*

15.40 Coffee break

Chair: Antonio SGAMELLOTTI (Linceo, Università di Perugia)

15.55 Savino LONGO (Università di Bari): *Montecarlo orbitals of confined atoms*

16.15 Danilo CALDERINI (ETH Zurich): *Nonadiabatic Ring-Polymer molecular dynamics*

16.30 Dario DE FAZIO (ISM-CNR, Roma): *Discretized harmonics for large angular momentum reactivity*

16.45 Dimitris SKOUTERIS (Scuola Normale Superiore, Pisa): *Chemical dynamics through propagation of localized orbitals*

17.00 Discussion and conclusions

ROMA - PALAZZO CORSINI - VIA DELLA LUNGARA, 10

Il convegno è organizzato con la collaborazione dell'Accademia Nazionale delle Scienze o dei XL
e del Dipartimento di Chimica, Biologia e Biotecnologie dell'UNIVERSITÀ DI PERUGIA

La partecipazione al convegno è libera, fino ad esaurimento dei posti disponibili. Si prega di segnalare la presenza
Segreteria del convegno: piemontese@lincei.it - www.lincei.it

Fino alle ore 10 è possibile l'accesso da Lungotevere della Farnesina, 10