



ACCADEMIA NAZIONALE DEI LINCEI e FONDAZIONE «GUIDO DONEGANI»

INTERNATIONAL CONFERENCE

STATISTICAL THERMODYNAMICS AND CHEMICAL KINETICS: FAR AWAY FROM EQUILIBRIUM

25-26 JUNE 2019

Organizing Committee: Vincenzo Aquilanti, Sergio Carrà, Tommaso Ruggeri

PROGRAMME

Celebrating 160 years from Arrhenius birthday and 130 years of remarkable success of his equation, open problems on its foundations and perspectives of future applications are under focus.

One of the tasks of statistical mechanics is to provide the connection between the mechanics of the systems at a molecular level and the macroscopic behavior of matter.

The ongoing work in the field of non-equilibrium thermodynamics is inspired by Onsager (Nobel 1968), Prigogine (Nobel 1977) and Kramers. In this context some recent results obtained by the extended thermodynamics theory of gases provide a derivation of the mechanics of continuum from the classical kinetic theory of gases (at a mesoscopic level): remarkable advances regarding chemical kinetics are directly inspired by Maxwell, a predictive theory of reaction velocities and a detailed formulation of the reactivity at low temperatures, accounting for modern experimental and molecular dynamics results.

The interdisciplinary and transversal character of the topic of this conference, from mathematics and physics to chemistry and the science of materials, dates back to more than a century ago. Historically, statistical mechanics intends to provide the connection between the mechanics of atomic and molecular systems and the macroscopic behavior, in order to arrive at a microscopic theory of thermodynamic functions, accepting the challenge launched in one of the famous problems of Hilbert and concerning the state of mathematics: in particular the sixth problem concerns the relationship between discrete reality at the atomic and molecular level and that of the macroscopic continuum.

Tuesday, 25 June: Mathematical Physics

14.00 Welcome address, Giorgio PARISI (Presidente dell'Accademia Nazionale dei Lincei)

14.15 Introduction by the Organizers

Chair: Francesco PEGORARO (Linceo, Università di Pisa)

14.30 Tommaso RUGGERI (Linceo, Università di Bologna): *New frontiers in non-equilibrium thermodynamics*

15.00 Masaru SUGIYAMA (Nagoya Institute of Technology): *A new link between kinetic theory and continuum thermo-mechanics*

15.30 Coffee break

Chair: Antonio SGAMELLOTTI (Linceo, Università di Perugia)

16.00 Constantino TSALLIS (Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro): *Beyond Boltzmann-Gibbs in physics, chemistry and elsewhere*

16.30 Annalisa MARZUOLI (Università di Pavia): *Discrete vs Continuum: quantum to classical via semiclassical*

17.00 Andrea LOMBARDI, Federico PALAZZETTI (Università di Perugia) – Mikhail B. SEVRYUK (Academy of Sciences, Moscow): *Statistics of energy partitions for many-particle systems*

Wednesday, 26 June: Statistical Thermodynamics

Chair: Tommaso RUGGERI (Linceo, Università di Bologna)

9.30 Ernesto P. BORGES (Universidade Federal da Bahia, Brazil): *From Boltzmann to non-Boltzmann distributions: strong to weak chaos*

10.00 Pier Luigi GENTILI (Università di Perugia): *Out-of-equilibrium chemical reactions in neuromorphic engineering*

10.30 Roger W. ANDERSON (University of California Santa Cruz): *Quantum reaction dynamics – Discrete algorithms*

11.00 Coffee break

Chair: Mario CAPITELLI (Università di Bari)

11.30 Massimo MORBIDELLI (ETH Zurich, Politecnico di Milano): *From polymer colloids to structural materials*

12.00 Paola DIOMEDE (Differ Institute, Eindhoven) - Savino LONGO (Università di Bari): *Fokker-Planck equation in chemical kinetics*

Chemical Kinetics

Chair: Annibale MOTTANA (Linco, Università di Roma Tre)

14.00 Sergio CARRÀ (Linco, Politecnico di Milano): Introduction

14.20 Tiziano FARAVELLI (Politecnico di Milano): *Combustion kinetics and the environmental challenges*

14.50 Enrico TRONCONI (Politecnico di Milano): *Hunting for elusive intermediates in the selective catalytic reduction of NOx: how a fundamental study may result in a new exhaust after-treatment technology*

15.20 Vincenzo AQUILANTI (Linco, Università di Perugia): Panel presentations and conclusions, including:

Dario DE FAZIO (CNR, Roma) – Simona CAVALLI (Università di Perugia): *Exact quantum dynamics and kinetics for cold and ultracold reactions down to the Wigner's limit*

Danilo CALDERINI (ETH Zurich): *Path integral approach for partition function calculations*

Valter CARVALHO-SILVA (Universidade Estadual de Goiás, Anápolis, Brazil) – Nayara DANTAS-COUTINHO (Universidade de Brasília): *Rate processes on the verge of the thermodynamic and the kinetic limits*

Conference organized in collaboration with

Accademia Nazionale delle Scienze detta dei XL, Rome - Università di Perugia

ROMA - PALAZZO CORSINI - VIA DELLA LUNGARA, 10

Segreteria del convegno: piemontese@lincei.it

La partecipazione al convegno è libera, fino ad esaurimento dei posti disponibili. Si prega di segnalare la presenza

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

Note the related event:

OBSERVATORY FOR ASTROCHEMICAL KINETICS AND RELATED ASPECTS

Accademia Nazionale delle Scienze detta dei XL, Villa Torlonia, Rome: 27- 28 June 2019

Organizers: Vincenzo AQUILANTI, Andrea LOMBARDI, Federico PALAZZETTI

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