



ACCADEMIA NAZIONALE DEI LINCEI  
FONDAZIONE «GUIDO DONEGANI»  
INTERNATIONAL CONFERENCE

## CONCEPTS IN CATALYSIS: FROM HETEROGENEOUS TO HOMOGENEOUS AND ENZYMATIC CATALYSTS

February 25-26, 2016

**Comitato ordinatore:** G. ALLEGRA, V. AQUILANTI, P. ASCENZI, V. BALZANI, V. BARONE, S. CALIFANO, S. CARRÀ, M. CATELLANI, D. GATTESCHI, G. GIACOMETTI, G. MARINO, F. MINISCI, G. PACCHIONI, M. PRATO, V. SCHETTINO, A. SGAMELLOTTI, R. UGO, G.G. VOLPI, G. ZERBI, A. ZECCHINA

**Comitato organizzatore:** S. CARRÀ, M. CATELLANI, G. MARINO, P. POLLESEL, R. UGO, A. ZECCHINA (Chair)

Catalytic processes (heterogeneous, homogeneous and enzymatic) are all based on the same principle, i.e. reduction of activation barrier associated with breaking and formation of chemical bonds at the active centers. Despite this common feature, heterogeneous, homogeneous and enzymatic catalysis have formed historically three separate branches of science that largely developed independently with modest reciprocal contamination. There is so space for trying to overcome these barriers, at least at the level of basic knowledge and information exchange. This is exactly the scope of the meeting at the Accademia dei Lincei that is designed for the whole chemical community and especially for PhD and Post Doc students belonging to the three different catalysis communities. The meeting content is not overlapping that of current scientific meetings, because it is focused on dissemination of basic information ranging from historical details to most recent and innovative directions.

### PROGRAMME

#### Thursday, 25 February

14.00 Welcome addresses

Introductory remarks by Adriano ZECCHINA (Linceo, Università di Torino)

Session 1 - Chair: Renato UGO (Linceo, Università di Milano)

14.15 Hans-Joachim FREUND (Fritz-Haber-Institut-Max-Planck-Gesellschaft, Berlin): *Models for heterogeneous catalysts: an approach at the atomic level*

15.05 Marta CATELLANI (Linceo, Università di Parma): *Homogeneous catalysis as an important tool for organic synthesis*

15.55 Vincenzo BALZANI (Linceo, Università di Bologna): *Photochemistry and photocatalysis*

16.45 Coffee break

Session 2 - Chair: Giuseppe ZERBI (Linceo, Politecnico di Milano)

17.15 Walter KAMINSKY (Universität Hamburg): *The discovery and evolution of metallocene based olefin polymerization catalysts*

18.05 Rinaldo PSARO (CNR - ISTM, Milano): *Homogeneous and heterogeneous catalysis: bridging the gap through surface organometallic chemistry*

#### Friday, 26 February

Session 3 - Chair: Paolo ASCENZI (Linceo, Università di Roma Tre)

9.30 Gianfranco GILARDI (Università di Torino): *Heme iron centres in Cytochrome P450: structure and catalytic activity*

10.20 Massimo COLETTA (Università di Roma Tor Vergata): *Modulation of catalysis in proteolytic enzymes*

11.00 Coffee break

Session 4 - Chair: Vincenzo BARONE (Linceo, Scuola Normale Superiore di Pisa)

11.30 Gianfranco PACCHIONI (Linceo, Università di Milano-Bicocca): *Modern electronic structure theory and catalysis: towards the simulation of complex problems in chemistry*

12.20 Silvia BORDIGA (Università di Torino): *Spectroscopic methods in catalysis*

Session 5 - Chair: Vincenzo SCHETTINO (Linceo, Università di Firenze)

14.30 Sergio CARRÀ (Linceo, Politecnico di Milano): *Peculiarities and perspectives of catalytic reaction engineering*

15.20 Ferruccio TRIFIRÒ (Università di Bologna): *Heterogeneous catalysis to realize a sustainable chemistry*

16.00 Paolo POLLESEL (ENI spa, San Donato Milanese): *The evolution of industrial catalysis in a complex oil refining scenario*

16.40 Closing remarks

ROMA - PALAZZO CORSINI - VIA DELLA LUNGARA, 10

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