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REGULAR ARTICLE

Theoretical and computational chemistry in Italy: an overview

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The development of new theoretical methods for the prediction and interpretation of physico-chemical observables has been accompanied—sometimes stimulated and sometimes dragged—by a wealth of new and sophisticated computational tools specifically devised by theoretically oriented chemists for molecular systems in different environments. At the same time, the rapid increase of computer power and the relative decrease of economic costs has lead to a capillary diffusion of computational techniques in many areas of chemical research, which were previously hardly touched by the extensive use of in silico approaches.

This indubitable progress has been made possible by the advances in the development of theoretical methods attuned to molecular problems, like quantum mechanical (QM) techniques using localized basis sets and rooted either on wave-function or density functional models. Further progress toward the treatment of complex systems is being done, thanks to the development of linearly scaling methods, multiscale approaches combining QM, molecular mechanics (MM), mean field (MF) models, effective Born–Oppenheimer and extended Lagrangian dynamical algorithms, sophisticated statistical mechanics approache to soft materials, and many others. Finally, one should not underestimate the importance of transparent, WYSIWYG-like implementations of many of these techniques, which is one of the main incentives for the spreading of commercial programs which are nowadays present in many experimental chemistry laboratories.

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More recently, the development of new solutions for high performance computing (HPC) has been based increasingly on the "scale out" principle. In essence, this amounts to the creation of metacomputing systems based on clusters, and specifically dedicated to large scale problems, which are typical of molecular sciences, e.g. prediction of structure and dynamics of materials at micro and nanoscale, interpretation of spectroscopic observables in condensed phases, or prediction of properties of biochemical systems.

In this general framework, the Italian chemistry community has proved to be alive, teeming with a number of interesting experiences. Relevant contributions come from several research groups which have further developed theoretical methods in physical, inorganic, organic, and pharmaceutical chemistry. Innovative ideas come from multi-disciplinary environments, like material, environmental, and life sciences. In a sense, the theoretical and computational chemistry sectors represent a success story, even taking into account the difficulties that fundamental research is encountering nowadays in Italy. The increasing need for intensive computational resources has lead to the participation of the chemistry community, mainly in the academic *milieu*, to national projects and computational centers. But until a few years ago most Italian chemists tended to be mere consumers of resources within pre-existing national and international projects. Today, there is a widespread demand of creative methods aimed at specific chemical applications. A political leadership of research enterprises is therefore required, which calls for a new role of the theoretical and computational chemists on an equal footing with experimental researchers, computational physicists, and so on.

More intriguing is the blossoming of local realities, at the level of single departments or groups of departments in several universities, which are constituted as *local virtual laboratories* combining the expertise and resources of different research groups. A first glance, even without a systematic analysis, allows to say that Italian Universities and Research Centres can count on (1) advanced competences for developing basic theoretical methods; (2) large participations to national and international projects, by tapping Computer Centres resources, and (3) intensive development of ad hoc software tools for chemical applications: we may for instance mention here the contributions of Naples and Pisa groups to the Gaussian project [1], or the development of dedicated software for crystalline solids carried on in Turin [2].

In the past, the theoretical and computational chemistry community in Italy was characterized by the presence of few and large research teams. In recent years, an evolution has taken place towards fragmentation into several small, geographically distributed teams, concentrating their activity on specific themes, often in close collaboration (when not fully integrated) with experimental groups. This trend could appear contradictory with the need of an integrated approach to the properties of complex systems (e.g. nanomaterials, biomolecules, etc.) which are at the heart of contemporary research in molecular sciences. This has stimulated the proposal of chemistry oriented geographically distributed networks, which could allow an effective integration both of computational resources and of specific high level skills.

The papers collected in the following pages witness, in my opinion, the remarkable level of theoretical and computational chemistry research in Italy and the wide geographic distribution of competences (see Fig. 1). A short summary, including leading references for the few research groups not represented in the present issue, can be of some general interest.

Starting from northern Italy, at the Università di Torino, an intense activity is dedicated to the development and application of an original approach to solids and surfaces based on localized basis sets. Universities in Lombardy are characterized by the development of new models for the structure and dynamics of complex systems at the Università di Milano, by computational studies in the fields of material and life sciences at the Università di Milano Bicocca, by the study of polymeric materials at the Politecnico di Milano [3], and by the elaboration and application of molecular dynamics approaches at the Università dell'Insubria [4]. In the Veneto region, the Università degli Studi di Padova is characterized by computational studies related to materials and organic molecules and by the development and application of methods based on stochastic approaches. At Trieste, we find intense activities devoted to the interpretation of spectroscopic parameters at the Università, and to numerical simulations of biomolecules at the *SISSA*. At the Università di Modena e Reggio Emilia, there is a traditional activity in the field of magnetic and photochemical phenomena, and the expansion of new original studies applied to biosystems and to complex materials, like glasses. At the Università di Parma, original methodologies are developed for modelling charge transfer processes in functionalized materials and spectroscopic processes in condensed phases. The Università di Ferrara is characterized by the development of quantum mechanical methods for excited electronic states, whereas research groups at the Università di Bologna are active in the fields of excited electronic states, radiation-matter interactions, vibro-rotational spectroscopy [5], nanomaterial properties, molecular dynamics, and Monte Carlo studies of liquid crystalline phases.

In central Italy, we find, in Tuscany, significant research activities for interpreting the properties of magnetic materials [6] and spectroscopic parameters via molecular dynamics at the Università di Firenze; contributions in the field of organic computational chemistry and nonadiabatic phenomena [7] at the Università di Siena, and above all the established research experiences at the Università and at the IPCF/CNR di Pisa, devoted to solvation effects in QM modeling, dynamics of excited states, spectroscopic parameters, and physico-chemical properties of biosystems. The Università di Perugia witnesses an established activity in the area of computational methods for kinetic processes and metallorganic systems. Finally, theoretical research devoted to reactive processes at quantum level is carried on at the Università la Sapienza di Roma, while more recent studies in biochemistry are present at the Università di Tor Vergata.

The advances of theoretical and computational chemistry in southern Italy are characterized by the research activities of several teams. We start from the Università del Sannio, where research is focused on statistical thermodynamics applications [8]; next we have the Università di Salerno, where activity regards the dynamics of excited states together with the properties and catalysis of polymeric materials [9,10]. Studies of reactive dynamics and development of improved density functionals are pursued at the Università di Bari [11] and at the NLL in Lecce, respectively. Properties of biomolecules are investigated at both the Università di Chieti [12] and the Università della Basilicata, while DFT methods are developed at the Università della Calabria.

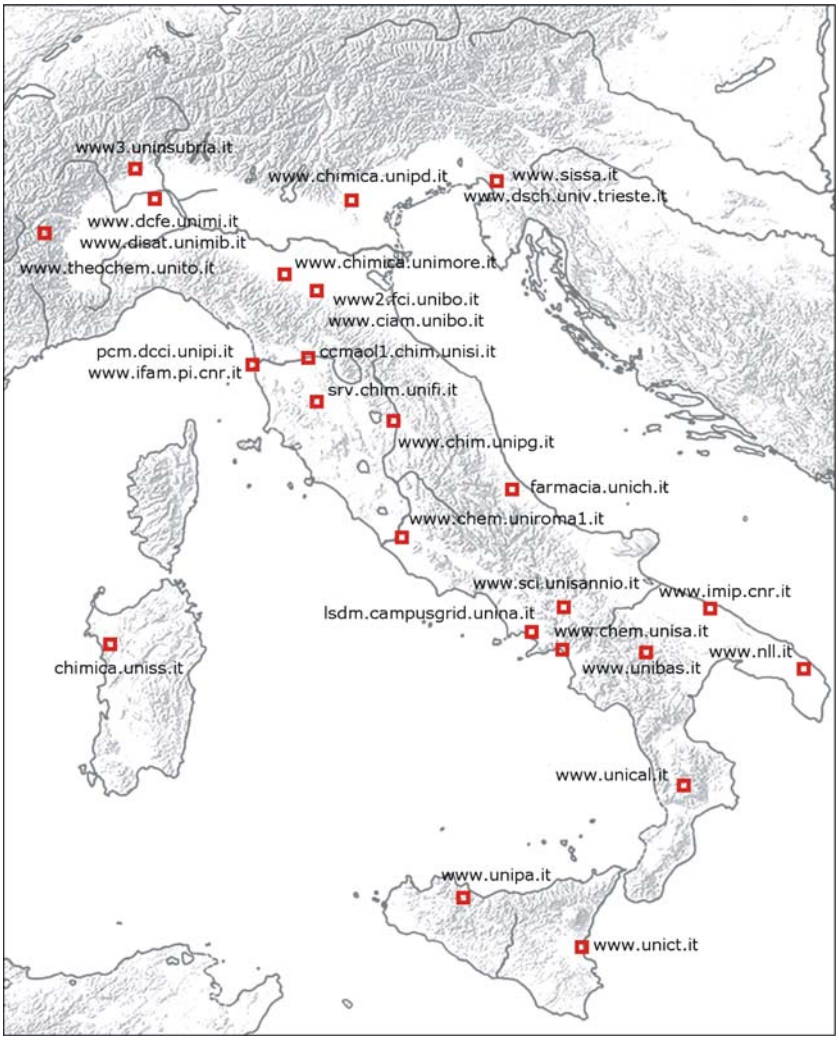

Fig. 1 Localization of the main theoretical and computational chemistry research groups in Italy

A particular attention is deserved by the school of the Università "Federico II" di Napoli, which has seen in the last years the development and validation of integrated computational approaches involving new density functionals and basis sets together with original methods for the static and dynamic treatment of complex systems in condensed phases. Large scale applications have been also performed for physico-chemical properties and processes of biochemical and technological interest. Finally, we recall the analysis of complex systems by quantum and statistical mechanical approaches at the Università di Catania [13], the studies of surface properties and of complex fluids by statistical approaches at the Università di Palermo [14,15] and the development of molecular dynamics methods applied to zeolitic systems at the Università di Sassari [16].

The identification of broad strategic lines of research can be of of great help, and their careful definition can only come from a dialectic strategic discussion. Several hot topics (e.g. extension of integrated approaches from different spatial to different temporal scales, improvement of computational tools for nano/microfluidic applications, development of quantum stochastic approaches, advanced modeling of molecular electronics, and spintronics) are definitely within the reach of the Italian theoretical and computational chemistry community, provided it will be able to increase its internal cohesion, and to find the necessary leverage to assume a more relevant role in the national and international scene. An important development along these lines can be mentioned regarding the methodological integration of traditional classical and quantum mechanical approaches with statistical methods. The first effort, which has brought forward effective tools for an integrated computational approach to the interpretation of spectroscopic parameters in condensed phases, is represented by the joint activities of the Laboratory for the structure and dynamics of molecules (LSDM) at the Università "Federico II" di Napoli, the theoretical chemistry group at the Università degli Studi di Padova, and the molecular

modeling laboratory (MML) of the IPCF/CNR in Pisa [17,18]. On these grounds, the same teams are organizing an innovative virtual laboratory, with the purpose of spreading the use of grid computing within the chemistry community, and of pooling different expertises: at present this new initiative, called virtual Italian laboratory for large-scale applications in a geographically-distributed environment (VILLAGE) [19] represents the backbone of a number of national and international projects. Finally, a lively activity of networking, organization, and coordination in this area is carried on by the Gruppo Interdivisionale di Chimica Computazionale della Società Chimica Italiana [20].

References

1. GAUSSIAN home page: www.gaussian.com
2. CRYSTAL home page: http://www.crystal.unito.it
3. Raos G, Allegra G (2000) J Chem Phys 113:7554
4. Fois E, Gamba A, Spano E (2004) J Phys Chem B 108:154
5. Puzzarini C (2005) J Chem Phys 123:024313
6. Adamo C, Barone V, Bencini A, Broer R, Filatov M, Harrison NM, Illas F, Malrieu JP, Moreira PR (2006) J Chem Phys 124:107101
7. Petrongolo C (2005) J Chem Phys 122:234315
8. Graziano G (2004) J Chem Phys 120:4467
9. Costabile G, Cavallo L (2004) J Am Chem Soc 126:9592
10. Milano G, Mueller-Plathe F (2005) J Phys Chem B 109:18609
11. Capitelli M, Colonna G, Esposito F (2004) J Phys Chem A 108:8930
12. Alberti M, Aguilar A, Lucas JM, Pirani F, Cappelletti D, Coletti C, Re N (2006) J Phys Chem A 110:9002
13. Brocca P, Cantù C, Corti M, Del Favero E, Raudino A (2002) Phys A 304:177
14. Barone G, Duca D Chem Eng J (2003) 91:139
15. Al-Anber Z, Bonet i Avalos J, Floriano MA, Mackie AD (2003) J Chem Phys 118:3816
16. Demontis P, Stara G, Suffritti GB (2004) J Chem Phys 120:9233
17. Barone V, Polimeno A (2006) Phys Chem Chem Phys 8:4609
18. Improta R, Barone V, Santoro F (2006) Angew Chem (in press)
19. VILLAGE home page: http://village.unina.it
20. GICC home page: http://www.soc.chim.it/grup_int_comp