

Topical collection of papers collected on the occasion of the XLI congress of the theoretical chemists of Latin expression (CHITEL 2015 - Torino - Italy)

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Theoretical and computational chemistry is a vibrant area of research and gathers a large community of scientists all over the world. Among them, the theoretical chemists who speak Romance languages (e.g., Italian, French, Spanish, Portuguese, Romanian, ...) play a crucial role by giving outstanding contributions to the development of such field.

Since 1969, this ever-growing community meets in a series of conferences denoted as CHITEL (for “Chimici Teorici di Espressione Latina” and “Chimistes Théoriciens d’Expression Latine” or QUITEL from “Químicos Teóricos de Expresión Latina” and “Químicos Teóricos de Expresão Latina”). Actually, this is not simply another congress on theoretical chemistry, rather the aim is to overcome the linguistic barrier and let participants speak their native languages because of the common origin from Latin, the language of science and philosophy for many centuries. With this idea in mind, CHI(QUI)TEL has then become a unique conference in which there are many official languages. Of course, the final scope is to promote new theories, models, methodologies and show applications and results of theoretical and computational chemistry to the entire Scientific Latin Community. CHI(QUI)TEL conferences then gather

people from Europe, Africa and Latin America. From 2003, the congress is organized in turn between the three continents.

In 2015, the XLI Congress of Theoretical Chemists of Latin Expression was held in Italy (Torino, July 26–31, 2015). This was the eighth edition in our country after Modena (1969), Cortona (1972), Stresa (1978), Alghero (1982), Roma (1990), Napoli (1999) and Cetraro (2008).

CHITEL 2015¹ took place in the beautiful city of Torino. Situated in the North of Italy, Torino was founded by Romans as *Julia Augusta Taurinorum* in the first century BC, but reached his most splendid period in the *Barocco* age under the Duchy of Savoy and Kingdom of Sardinia. Soon after, Torino became the first capital of Italy. Although, Torino is not as renowned and famous as other Italian cities, it is a very fascinating town with a hidden charm. Admittedly, Torino was a nice surprise for all participants and accompanying persons.

More than 200 delegates were hosted at the conference center “Torino Incontra” located in the city center (see Fig. 1). We had 5 plenary speakers (W. Andreoni (Switzerland), B. Mennucci (Italy), T. de Castro Ramalho (Brasil), M. Sodupe (Spain) and A. Tkatchenko (Germany)), 16 keynote talks, 30 oral communications and 12 flash presentations (see footnote 1). The geographic distribution of the 63 speakers is shown in Fig. 2.

Along with the 63 oral contributions, there were 160 posters subdivided in three poster sessions. The congress covered many exciting topics from new developments in electronic structure theory to molecular structure, interaction and reactivity and from time-dependent phenomena and spectroscopy to biochemical theory and computations, and multiscale modeling of bulk and nano-materials. In

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This topical collection is dedicated to the memory of our colleague and friend Roberto Orlando, one of the organizers of the congress and guest editor of this topical collection, who passed away prematurely on April 2016.

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¹ www.chitel2015.org.

Fig. 1 A picture of some of the participants of the CHITEL 2015



Fig. 2 Geographic distribution of the speakers of the CHITEL 2015

addition, we had a special session on High Performance Computing sponsored by the PRACE initiative.² Selected speakers who work in the development of programs for both molecular and solid state modeling were invited to

² www.prace-ri.eu.

show how theoretical and computational chemistry can be done on *tier-0* machines. We also had a keynote talk by K. Ruud (Norway) from PRACE board of directors (see footnote 2).

In this special issue, we are delighted to present a collection of 39 articles originated from authors who also delegates at the XLI Congress of Chemists of Latin Expression

held in Torino. It is a pleasure that this topical collection is hosted on Theoretical Chemistry Accounts (TCA). This journal has a long tradition in the theoretical chemistry field and a special link to Latin. Indeed, it was formerly named as *Theoretica Chimica Acta* and was one of the few journals that accepted articles written in Latin.

The guest editors wish to thank the TCA Editors in Chief Carlo Adamo and Ilaria Ciofini, and the editorial staff. We also thank our colleagues who kindly contributed to this special collection and all the referees who generously gave their time and expertise.

The congress was intended to promote the exchange of ideas, strategies and techniques in theoretical and computational chemistry, trusting that all international and national co-operations born during the congress could be fruitful. We believe this topical issue shows how our hopes have been fulfilled.

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