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Editorial
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Molecular Simulation in Latin America: Coming of Age

Latin America has a long tradition in theoretical chemistry.[1] What appears to be the first theoretical chemistry paper fully thought and developed in Latin America was published in 1964 by Brazilian−Argentinian researchers.[2] However, it took nearly two decades for what is now recognized as molecular simulation to bloom in the intellectually diverse but often politically tumultuous landscape of Latin America (Figure 1).

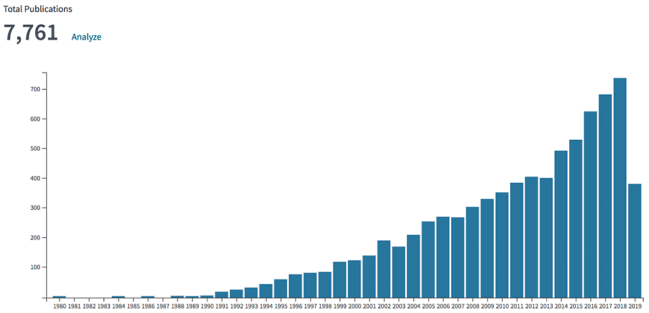

Figure 1. Growth of publications in the field of molecular simulations in Latin America. The data was retrieved by querying the core collection of the Web of Science for the term "molecular simulation" combined to all Latin American countries.[3]

The new field was deeply rooted in quantum chemistry and theoretical physics and rapidly branched out to include a broad spectrum of topics in (bio)chemistry, (bio)physics, and chemoinformatics from a molecular level perspective.

In the last 30 years molecular simulation in Latin America has not only matured and diversified into different areas but has found its own identity as a community. The establishment of research groups by scientists who returned home after graduate school and postdoctoral education abroad, the creation of molecular simulation schools intended for specialized training of undergraduate and graduate students, and continuous funding of cooperation networks greatly contributed to the progress and expansion of the molecular simulation field in Latin America.[4,5] However, greater scientific integration among researchers in Latin America remains a hurdle (Figure 2).[6] The available data for the number of collaborative publications between South American countries is rather low when compared to joint publications with the United States, the main international collaborator in the region.[6] One route to increase collaboration between Latin American researchers in molecular simulation is through the creation of grassroots-level initiatives such as the South American Initiative on Molecular Simulation (SAIMS).[7] SAIMS was established in 2015 with the goal of fostering collaborative work between members, sharing advanced knowledge to enhance scientific research in the region, promoting and coordinating advanced training to nurture human capital, and supporting the development of infrastructure to empower research in the field of molecular simulations. It is currently made up of research groups from 10 different South American countries (Argentina, Bolivia, Brazil, Chile, Colombia, Ecuador, Paraguay, Peru, Uruguay, and

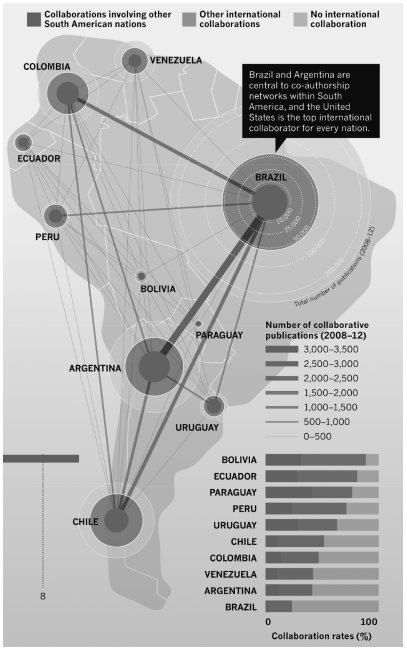

Figure 2. Number of collaborative publications between South American-based research groups from 2008 to 2012 [Reprinted from ref 6 with permission. Copyright 2014. Nature Publishing Group].

Venezuela). In the spirit of such grassroots drive, the *Journal of Chemical Information and Modeling* (JCIM) has put forward a proposition for a special issue dedicated to molecular simulation in Latin America.

Although the number of publications in JCIM from researchers in Latin America is increasing in recent years, this number remains low if compared to the USA, Germany, China, and England (Figure 3). Together Argentina, Brazil, Chile, and Mexico authored 3% of the total of number of publications in JCIM in the last 10 years. JCIM strives to be a publishing hub for greater integration of the Latin American

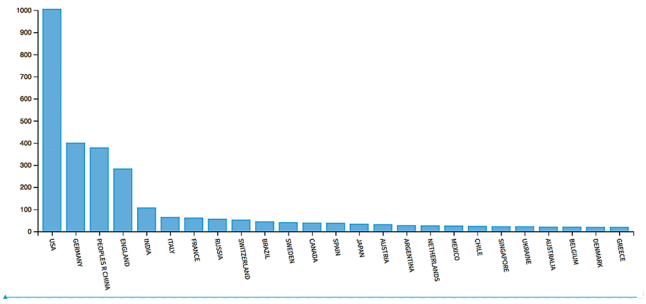

Figure 3. Number of publications in JCIM per country. The data was retrieved by querying the core collection of the Web of Science for the term "Journal of Chemical Information and Modeling" between 2009 and 2019.[3]

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scientific community while promoting the highest-quality standards of scientific research in chemical information and modeling. To achieve this aim, JCIM will launch a special issue on **Molecular Simulation in Latin America: Coming of Age**. We invite researchers from Latin American institutions to submit a review, perspective, article, or letter on the many facets of molecular simulations including the representation and computer-based searching of chemical databases, molecular modeling, computer-aided molecular design of new materials, catalysts, or ligands, development of new computational methods or efficient algorithms for chemical software, and biopharmaceutical chemistry including analyses of biological activity and other issues related to drug discovery. The submission deadline is September 15th, and the special issue will be launched in January 2020. We hope to have you joining us.

Thereza A. Soares
Habibah A. Wahab

AUTHOR INFORMATION

ORCID

Thereza A. Soares: 0000-0002-5891-6906
Habibah A. Wahab: 0000-0002-8353-8679

Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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