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Editorial

Computational Chemistry in the Global South: A Latin American Perspective

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Computational science has transformed our ability to explore chemical, physical, and biological processes at the molecular level. These advances have led to breakthroughs that were once unimaginable. Sophisticated physical methods, combined with increasing computational power, have accelerated progress in computational chemistry and biology. The rapid rise of artificial intelligence has further enhanced this powerful toolbox, enabling extraordinary achievements in biomedicine, bioengineering, and materials science.

Diversity is a cornerstone of innovation, fostering new perspectives and driving scientific progress. Ensuring inclusive representation is crucial for addressing socially relevant challenges, such as regional health, environmental sustainability, and industrial development, in both basic and applied research. Achieving this level of inclusivity requires a commitment to international mentorship, equitable recruitment, and sustained funding. These efforts should offer support for underrepresented groups, including gender minorities, diverse ethnic communities, and scientists from less-developed regions, empowering them to contribute meaningfully to the global scientific landscape.[1]

The term *Global South* refers to countries in Africa, Latin America, Asia, and Oceania.[2] Over recent decades, research output from the Global South has grown significantly. However, disparities remain when compared to the United States and Europe. Latin America, for instance, would benefit greatly from sustained scientific support and regional collaborations. Five years ago, inspired by a series of scientific meetings in Latin America, we launched an initiative to showcase the region's progress in the computational research. This effort culminated in a special issue of the *Journal of Chemical Information and Modeling* (*JCIM*),[3,4] featuring 59 research articles that have garnered nearly a thousand citations. Since then, research contributions from Latin American institutions to *JCIM* have tripled, reaching 35−40 papers per year with consistently strong citation rates (Figure 1). Although challenges remain, such as Latin America holding just 3% of the world's supercomputer power,[5,6] this progress reveals the region's immense potential. Inclusive editorial policies, international collaboration, and expanding resource-sharing networks can help bridge these gaps. Latin America's growing contributions prove that, with the right support, it can become a key player in global scientific progress.

The *Journal of Chemical Information and Modeling* (*JCIM*) and the *Journal of Chemical Theory and Computation* (*JCTC*) are excited to announce a joint Special Issue on Computational Chemistry in the *Global South: The Latin American Perspective*.

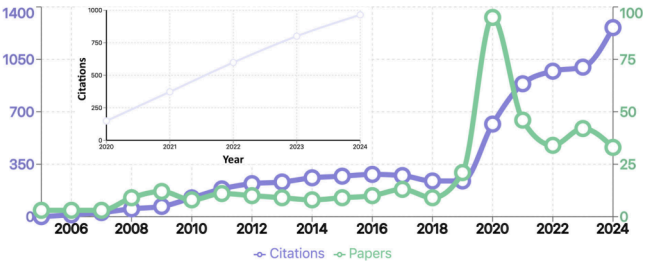

Figure 1. Web of Science metrics for *JCIM* papers authored by researchers affiliated with Latin American institutions. The inset shows the cumulative number of citations received by the manuscripts published in the *JCIM* special issue *Molecular Simulation in Latin America: Coming of Age*[3,4] in 2020.

This special issue welcomes cutting-edge research from authors affiliated with Latin American Institutions and within the scopes of both journals. All manuscript types published by *JCIM* & *JCTC* are eligible. To maintain and advance this momentum, contributions should focus on new computational methods, chemical theories, computational algorithms, and advanced applications to complex chemical systems as innovative methodologies and theoretical developments are key to pushing the frontiers of computational science and delivering transformative insights into complex molecular phenomena. For details on the scopes, manuscript types, and submission guidelines of the two journals, please visit the Web sites of *JCIM* & *JCTC*. Submissions are open through **October 30th, 2025**. All manuscripts will undergo peer review to ensure they meet the high scientific standards of *JCIM* & *JCTC*. Accepted manuscripts will be published online as soon as possible and included in the next available issue. All publications will be gathered into a webpage dedicated to the Special Issue and widely promoted. We look forward to showcasing the best of Latin American computational chemistry.

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Notes

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