J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Fifty Years of Molecular Simulations at UAM and in Mexico

Edgar Núñez-Rojas[1], Alexander Pérez de la Luz[2], Humberto Saint-Martin[3], José Alejandre[2*]

[1]CONAHCyT-Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa. Av. San Rafael Atlixco 186, Col. Vicentina, 09340, Ciudad de México, México.
[2]Departamento de Química. Universidad Autónoma Metropolitana-Iztapalapa. Av. San Rafael Atlixco 186, Col. Vicentina, 09340, Ciudad de México, México.
[3]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Campus Chamilpa, 62210 Cuernavaca, Morelos, México.

***Corresponding author:** José Alejandre, email: jra@xanum.uam.mx

Received May 24th, 2024; Accepted July 21st, 2024.

DOI: http://dx.doi.org/10.29356/jmcs.v68i4.2291

Abstract. Molecular simulation methods are the bridge between molecular interactions and the macroscopic properties of matter. The equations of statistical mechanics give the probabilistic method of Monte Carlo while those of Newton are the bases of Molecular Dynamics, which is deterministic. A molecular simulation predicts the movement of molecules and hundreds of physicochemical properties can be obtained to understand its behavior at different thermodynamic conditions. The molecular simulation methods were developed in the 1950s in United States of America and in the 1980s in Mexico, **where *Universidad Autónoma Metropolitana* (UAM)** was a pioneer. It is a multidisciplinary field that involves mathematicians, chemists, physicists, engineers from different disciplines, biologists, computer scientists, etc. Supercomputers have played an important role in its development. Currently, the United States, China and the European Community have everyone more than 100 supercomputers in the TOP500 ranking, while Canada and Brazil have 10, Spain 3, Argentina 1 and Mexico none. These resources allow increasing the training capabilities, the production of research articles, the organization of academic events, etc.
In this work, we make a review of the development of molecular simulations at UAM and in Mexico. The diffusion and promotion of this research field has been undertaken by academic leaders from several universities. We have organized **12 Molecular** Dynamics Workshops nationwide to teach and put the basic concepts into practice and **13 international Meetings on Molecular Simulations** to discuss the state of the art in research projects. The number of articles in molecular dynamics grows exponentially over time; in 2023, more than 250,000 were published worldwide. Mexico contributed 10 % and the UAM 10 % of those published in Mexico. There are more than 32 Mexican leaders living in Mexico who have published around 120 articles with at least 100 citations, according to Web of Science. About 70 % belong to the National System of Researchers at levels III and Emeritus. The research lines range equations of state in liquids, phase equilibrium, development of simulation methods and force fields, polar fluids, electrolytes, colloids, polymers, drug/protein interaction, protein folding, among others.
Keywords: Molecular simulations; molecular dynamics; Monte Carlo; simulation in Mexico; workshop and meetings; force fields; condensed matter; supercomputing.

Resumen. Los métodos de simulación molecular son el puente entre las interacciones moleculares y las propiedades macroscópicas de la materia. Las ecuaciones de la mecánica estadística dan el método probabilístico de Montecarlo mientras que las de Newton son las bases de la Dinámica Molecular, que es determinista. Una simulación molecular predice el movimiento de las moléculas y se pueden obtener cientos de propiedades fisicoquímicas para comprender su comportamiento en diferentes condiciones termodinámicas. Los métodos de simulación molecular se desarrollaron en la década de 1950 en Estados Unidos de América y en la década de 1980 en México, **donde la Universidad**

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Autónoma Metropolitana (UAM) fue pionera. Es un campo multidisciplinario que involucra a matemáticos, químicos, físicos, ingenieros de diferentes disciplinas, biólogos, informáticos, etc. Las supercomputadoras han jugado un papel importante en su desarrollo. Actualmente, Estados Unidos, China y la Comunidad Europea cuentan con más de 100 supercomputadoras en el ranking TOP500, mientras que Canadá y Brasil tienen 10, España 3, Argentina 1 y México ninguno. Estos recursos permiten incrementar las capacidades de formación, la producción de artículos de investigación, la organización de eventos académicos, etc.
En este trabajo hacemos una revisión del desarrollo de simulaciones moleculares en la UAM y en México. La difusión y promoción de este campo de investigación ha sido llevada a cabo por líderes académicos de varias universidades. Hemos organizado **12** Talleres de Dinámica Molecular a nivel nacional para enseñar y poner en práctica los conceptos básicos y **13 Simposios internacionales sobre Simulación Molecular** para discutir el estado del arte en proyectos de investigación. El número de artículos sobre dinámica molecular crece exponencialmente con el tiempo; en 2023, se publicaron más de 250.000 en todo el mundo. México aportó el 10 % y la UAM el 10 % de los publicados en México. Hay más de 32 líderes mexicanos viviendo en México que han publicado alrededor de 120 artículos con al menos 100 citas, según Web of Science. Alrededor del 70 % pertenece al Sistema Nacional de Investigadores en los niveles III y Eméritos. Las líneas de investigación abarcan ecuaciones de estado en líquidos, equilibrio de fases, desarrollo de métodos de simulación y campos de fuerza, fluidos polares, electrolitos, coloides, polímeros, interacción fármaco/proteína, plegamiento de proteínas, entre otras.
Palabras clave: Simulación molecular; dinámica molecular; Monte Carlo; simulación en México; talleres y simposios; campos de fuerza; materia condensada; supercómputo.

Theory and molecular simulations to understand matter

It is well recognized that the father of molecular simulations is Professor Bernie J. Alder (1925-2020), from the University of Lawrence Livermore National Laboratory in the United States of America. He published the first works in the mid-1950s on Monte Carlo and Molecular Dynamics applied to hard spheres systems [1]; he predicted a first order solid-liquid phase transition driven by entropic effects, also, that the phase diagram of this system did not contain a liquid-vapor equilibrium. He developed his simulations on the fast computer on those days, UNIVAC and then IBM, which had two CPUs and one processor. The weight of the machine was around 52 tons. A smart phone today has more computer power than NASA´s supercomputer in 1960. This paper has more than 1800 citations according with Web of Science (WofS) and is still being cited. Professor Alder received the National Medal of Science from President Barack Obama in 2009.

Professor Jorge Barojas was the first Mexican that published an article on molecular dynamics from his PhD research with Professors D. Levesque and B. Quentrec in France in 1973. They used the Lennard-Jones potential to simulate diatomic homonuclear liquids and compared their equation of state and their structure factor with experimental values of nitrogen finding a good agreement [2]. Professor Barojas returned to Mexico and, though he did not work anymore in molecular simulations field, he is regarded as a pioneer in science outreach in Mexico, an activity that in his time was not popular between his colleagues, but time has shown the relevance of his work in promoting specific vocation, including editorial production on this area.

Professor Gustavo A. Chapela obtained his PhD with Professor John S. Rowlinson at Imperial College London, United Kingdom, and published two **seminal** articles about the liquid-vapor interface also using the Lennard-Jones potential. In these works, they applied Monte Carlo and Molecular Dynamics with 255 particles to obtain the coexisting densities and surface tension at temperatures from the triple to critical points. Binary mixtures were also studied [3,4]. The latter paper has more than 350 citations and it is still cited. The results were obtained in a CDC supercomputer of those days. Professor Chapela returned to Mexico to work at the Physics Department at UAM-Iztapalapa where he began to promote molecular dynamics.

In those years UAM had a CDC fast computer but it was used, mainly, for administrative tasks, not for research. The computer was in the *Rectoría General*, in the north of Mexico City, near to *Toreo de Cuatro Caminos* forum. The bachelor´s degree in computer science was created in early 80s. The students developed their Fortran programs using card punchers and typed cards as those shown in Fig. 1. The same tools were used

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

by researchers. The cards had to be submitted from UAM-Iztapalapa to ***Rectoría General*** **building** to compile the program. The compiled version was returned to UAM-Iztapalapa to correct the errors.

Fig.1. Card puncher (left panel) and card for the sum X + Y in a fortran program (right panel).

The cards sometimes were sent on motorcycles from UAM-Iztapalapa to *Rectoría General*. In some cases, it is said that the driver dropped the cards and rearranged them inside the box as he could but in disorder, so that they could be compiled. In those cases, when the list of the compiled version of the program was returned to the author, it turned out that it contained more errors than in the previous version.

Gustavo Chapela: founding father of molecular dynamics at UAM and in Mexico

The UAM-Iztapalapa is pioneer in the development and application of molecular simulation methods in Mexico. Professor Chapela and his group published in 1980, in **Spanish**, an internal report for the *División de Ciencias Básicas e Ingeniería* of UAM-Iztapalapa. This was the first simulation carried out in Mexico. The cover of this internal report is shown in Fig. 2.

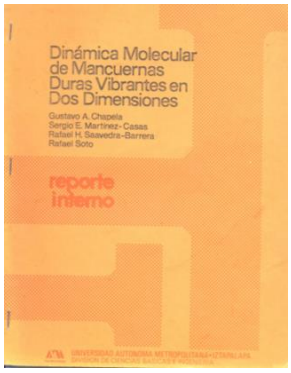

Fig. 2. Internal report titled *Dinámica Molecular de Mancuernas Duras Vibrantes en Dos Dimensiones* by **G. A. Chapela, S. E. Martínez-Casas, R. H. Saavedra-Barrera and R. Soto.**

Professor Chapela and Sergio E. Martínez-Casas published the first molecular simulation article made in Mexico in an international Journal in 1983 [5].

In the 80s and 90s, research performed in Mexico around Simulation and Molecular Theory, (**SMT**), was mainly based on the statistical mechanics methods. It involved predicting thermodynamic, dynamic and

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

structural properties from **potential models**, such as hard spheres, square well, Lennard-Jones or Yukawa **interactions**. The results of molecular simulations were used to both, testing statistical mechanics theories and understanding the effect that molecular interactions have on macroscopic properties. Systems studied included liquids, electrolytes, colloids, polymers, among other applications.

It is important to keep the community together, therefore, several efforts were made to promote theory, simulation, and experimental work. The Winter Meeting on Statistical Physics, where **Professors Fernando del Río and Leopoldo García-Colín were promotors**, has been organized continually for more than 50 years. The Meeting on Complex Fluids in San Luis Potosí was pioneered by Professor Magadaleno Medina Noyola and his group and it has been organized for more than 30 years. Professor José Alejandre organized in 1998 an international meeting at the *Instituto Mexicano del Petróleo* in Mexico City, the event titled *Simposio de Simulación Molecular y Técnicas Experimentales en Problemas del Petróleo* was attended for more than 200 participants.

The importance of the **SMT** topic lies in the fact that there is currently better knowledge about the role played by molecular interactions, and it is viable to use the methodology to generate new knowledge and support technological innovation. In this sense, in industrialized countries, as a development strategy, research centers that use **SMT** methodologies have already been created. Explaining the physical phenomena of molecular systems from the interactions of the constituent atoms based only on experimental data is incomplete because, in general, these data lack the resolution needed to attain atomistic detail. Therefore, in many cases, this is carried out through trial and error, which is expensive and requires a long time.

Nowadays, the interactions can be obtained with quantum mechanics where electrostatic and polarization contributions can be included with or without chemical reactivity. Some of the computational methodologies are classical and *ab initio* molecular dynamics, Monte Carlo, mesoscopic dynamics, QM/MM, etc.

Currently, thanks to the enormous advance in supercomputer development technology and molecular simulation methods, a wide range of complex problems in chemistry, physics, biology and engineering can be studied and understood at the molecular level. It is well known that the forces between atoms and molecules determine the physical and chemical properties of matter. With molecular simulation methods, the movement of molecules and the way they interact are studied. The application of these methods has allowed us to have a better knowledge of the role that these forces play in the description of a large number of physical phenomena. It is estimated that they can impact the development of areas such as health (design of better drugs), energy (materials to transport and store fuels more efficiently, biofuels, renewable materials such as lithium batteries, solar cells) and the environment (friendly solvents, separation and storage of contaminants).

National Prizes of Sciences and Arts in Mexico

In Mexico, 5 national prizes in physical-mathematical sciences have been awarded to researchers who have made important scientific contributions in the field of statistical mechanics and some of them also in molecular simulations.

Leopoldo García Colín-Scherer **- National Prize for Sciences and Arts 1988.** He was interested in the study of statistical physics of nonequilibrium systems, nonlinear irreversible thermodynamics and its astrophysical and cosmological applications, hydrodynamics, superfluidity, and the glass transition. He was founder and professor of the *Escuela Superior de Física y Matemáticas* in *Instituto Politécnico Nacional* (IPN) in 1961, *Universidad Autónoma de Puebla* in 1964, the *Facultad de Ciencias* UNAM in 1967, Physics and Chemistry departments of UAM-Iztapalapa in 1974; he was subdirector of the *Instituto Mexicano del petróleo* in 1967, he was also researcher at the Nuclear Center Salazar (1966) and at the *Instituto de Investigaciones en Materiales* in UNAM in 1984. He published 52 articles and the most cited (*Physics Reports 465 (2008) 149–189*) has 104 citations.

Alberto Robledo Nieto **- National Prize for Sciences and Arts 2008.** He simultaneously studied Chemical Engineering, Chemistry and Physics at UNAM. He completed his PhD in Statistical Mechanics at the Department of Theoretical Physics at the University of Saint Andrew, in Scotland. His valuable, original and varied contributions to knowledge in areas of physical chemistry within the framework of statistical mechanics stand out. For around 40 years he has taught courses in *Facultad de Química* and *Facultad de Ciencias* in UNAM. He has also developed the infrastructure used by the research groups of the thermophysics laboratory of *Facultad de Química* in UNAM. His specialty is statistical physics and his research frequently involves the description of

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

phase transitions in condensed matter. He has published around 200 articles and the most cited (*Physical Review E 66 (4), (2002) 045104*) has 153 citations.

Marcelo Lozada-Cassou **- National Prize for Sciences and Arts 2010.** His scientific contributions can be divided into two groups: a) Development of the fundamental theory of many-body physics; b) Prediction of new physicochemical phenomena, which have subsequently been experimentally verified by other researchers. His work on the electrical double layer is widely recognized as pioneering for understanding the structure of inhomogeneous fluids. He also contributed to the development of fluid transport theories. His PME theory contributed to the understanding of charged particle electrophoresis, and significantly improved the theory of Wirsema, O'Brien and White. His works have been published in major and widely recognized textbooks for students; graduates in physical chemistry. It should be noted that he has generated basic scientific ideas that he later transformed into 19 international and 12 national patents currently in the process of industrial development at the IMP, under the premise of the connection between first-class science and effective attention to priority problems of the country. He has published 121 articles and the most cited (*Nanotechnology 13 (2002) 495–498)* has 197 citations.

Magdaleno Medina Noyola **- National Prize for Sciences and Arts 2013.** He has been focused on the study of the physicochemistry of complex fluids. His contributions have been at the forefront in the description of such properties in the context of colloidal suspensions and micellar solutions. His work includes important and diverse contributions both to theory in general and to the understanding of specific phenomena, including the theory of liquids and ionic fluids, works that were pioneers in a topic that currently constitutes a topic of great interest in physics. statistics. Regarding his contribution to the development of academic infrastructure, the formation of Statistical Physics groups at *Centro de Investigación y de Estudios Avanzados* (CINVESTAV) stands out in the 1980s. In 1984, he restarted the Advanced Summer School in Physics. He formed the Statistical Physics and Physiochemistry of Complex Fluids group of the *Instituto de Física* in *Universidad Autónoma de San Luis Potosí*, from which a small and excellent group of researchers emerged who have obtained important support, such as emerging fields and links with industry of the oil. He also highlights the Statistical Physics and Complex Fluids group at the University of Sonora. He has published 121 articles and the most cited (*Phys. Rev. Lett. 60, 2705. 1988)* has 196 citations.

Fernando del Río Haza **- National Prize for Sciences and Arts 2015.** His research has contributed to the knowledge of the structure and thermodynamics of this system. His main research contributions form a coherent set, and can be separated into four groups: 1) the so-called square well model systems, 2) the theoretical equation of state of real substances, 3) the effective intermolecular potentials, and 4) the systems with Coulomb interaction. He is a researcher trainer with the direction of more than 40 doctoral, master's and bachelor's theses. Likewise, his teaching activity is manifested in several books and more than 150 courses taught. He has published 87 articles and the most cited (*Molecular Physics, 100(15). (2002),2531–2546)* has 103 citations.

All of them have promoted the development of science along the Mexican country. The information used to describe the activities that granted them the prize was taken from https://www.gob.mx/sep/acciones-y-programas, https://www.webofscience.com and https://scholar.google.com.

The birth of a molecular simulation group in Mexico

Over the years the number of researchers and students in the molecular simulation field has increased. In 2009, Professor José Alejandre and Roberto López Rendón (†), his PhD student, organized the first Molecular Simulation Symposium at UAM-Iztapalapa. Professor Alejandre, who got his PhD under the supervision of Professor Chapela, was working in the Chemistry Department of that institution. The objective of the symposium was to promote the molecular simulation field among the Mexican community and learn about the state of the art in both methods and applications. The lectures were given by Mexican experts in theory of liquids and the classic methods of Molecular Dynamics and Monte Carlo. All the invited colleagues agreed to participate, and the event was held in one day. The talks were given in Spanish. The speakers were Professors Fernando del Río (UAM-Iztapalapa), Minerva González-Melchor (BUAP), Jorge López-Lemus (UAEMex), Gustavo A. Chapela (UAM-Iztapalapa), Pedro Orea (IMP), Ana Laura Benavides (UG), Humberto Saint-Martin (UNAM), José Alejandre (UAM-Iztapalapa), Gerardo Odriozola (IMP), Roberto López-Rendón (UAMex) and Gerardo Pérez (UAMC). The picture of the participants taken in the Cuicacalli Room is shown in Fig. 3.

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

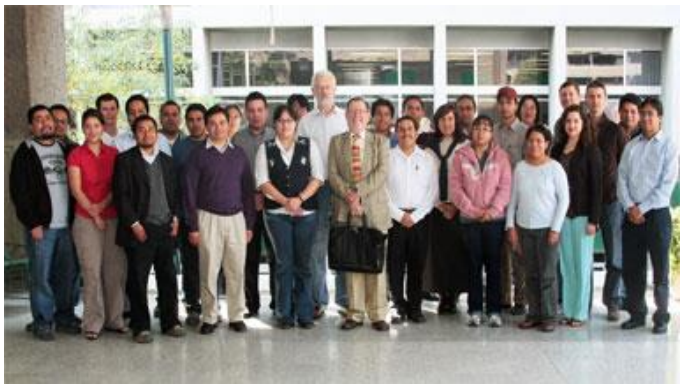

Fig. 3. Participants at the first Molecular Simulation Symposium at UAM-Iztapalapa in 2009.

Given the great success with students and researchers in the field of molecular simulations in the first Symposium, Professor José Alejandre proposed to organize a Workshop in the summer and a Meeting on winter. In the Workshops, the basic aspects of the methodology and the use of highly parallel programs such as GROMACS, DL_POLY, LAMMPS and NAMD should be taught by national researchers who are experts in the field of molecular simulation. Participating students should carry out the computer experiments on their own computers. More information about the Workshops **is given** below.

International meetings on molecular simulations in Mexico

The main purposes of the Meeting are to promote research in molecular simulation in Mexico and establish collaborations with both, national and international researchers. Also, the Meeting is an opportunity that allows us gathering a group of people to share their research and knowledge about molecular simulations. The Meeting offers a series of lectures in which experts from Mexico and other countries present results and accomplishments of their research. There is also a poster session where members of the community, students and researchers, can discuss their results. The Organizing Committee has taken the initiative of gathering both academic and industrial experts in a common place, the aim of these meetings is to establish and understand problems which industry deal with in order to find out how molecular simulation methods can contribute to resolving them. Nowadays, with the great advances in computer technology and simulation methodologies, it is important for the productive sector that academics know the troubles in the industry and that industry knows the reaches of molecular simulations. In Fig. 4 a picture of the participants of the second Molecular Simulation Meeting at UAM-Iztapalapa in 2010 is **shown**.

Fig. 4. Participants at the second Molecular Simulation Meeting at UAM-Iztapalapa in 2010.

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

The main objectives of the Meeting have been:

1) Promote research in the field of Molecular Simulation in Mexico and establish scientific collaborations with national and international researchers.
2) Motivate graduate and postgraduate students to discuss their research.
3) Promote the mobility of students and researchers between different institutions at a national and international level.
4) Establish a national/international molecular simulation network.
5) Grant recognition every two years to a national researcher in the field of Molecular Simulation.

The number of national researchers, undergraduate and graduate students has increased with time. Noticeably in recent years, this has been reflected in the increase in research papers published in high-impact international journals. Given the high academic level of the Meetings, a special volume was published in the Journal of Molecular Liquids in 2012 with research results presented at the Meeting. There is also a poster session where students at different levels and young researchers participate. In 2015, The Journal of Chemical Theory and Computation awarded $250 usd to each of the three best posters of the Meeting thanks to the initiative of Professor Julián Tirado-Rives and his wife, MsC Patricia Morales de Tirado, for get these important supports. This award helped raise the level of content of around 40 works presented. The jury has been made up of national and international researchers. The winners are normally graduate students. The award, **academic and economic**, is a good incentive to continue working in this field. The names of the winners and the title of their works are given in Table 1. In Fig. 5 the winners of the Poster session in the 7th Meeting on Molecular Simulations in 2015 can be seen.

Table 1. Name of the poster winners in the Meetings of Molecular Simulations from 2015. The years 2020 and 2021 the Meeting was not organized because the COVID pandemia.

Meeting	Name	Institution	Title of the work
7th in 2015	Sandra Guadalupe Hernández Ríos	UASLP	A comparison of different force fields for calculating [C_4MIM][BF_4] vapor-liquid equilibria using molecular simulations
	Janett Torres Ruíz	IPN	*Evaluación in silico de posibles inhibidores terapéuticos contra el virus de la rabia*
	Alexander Pérez de la Luz	UAM-Iztapalapa	Re-parameterizing a force field for formamide molecule
8th in 2016	María del Rosario Eustaquio-Armenta	BUAP	The line tension of an ionic fluid
	Sandra Acebes	Barcelona Supercomputing Center, Spain	In silico Rational Enzyme Engineering of Manganese Peroxidase through Biophysical and Biochemical Modeling
	Jorge Alberto Aguilar-Pineda	UAM-Iztapalapa	Reparameterization of force fields for nitrogen compounds in liquid phase
10th in 2018	Ana Beatriz Salazar Arriaga	IIM-UNAM	Desorption of alkanes from a graphite surface produced with different surfactants: anionic and betaine by Molecular Dynamics
	Minerva Valencia	IIM-UNAM	CO_2 capture using Na-Y siliceous type zeolite modified with SDS
	Jonatan Isaí Sánchez Sánchez	BUAP	Computational modeling of boron nitride nanotube applied to biomedicine

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Meeting	Name	Institution	Title of the work
11th in 2019	Laura María Castro González	UNAM	Design of multifunctional antioxidants derived from sesamol
	Valeria García Melgarejo	UAM-Iztapalapa	Development of force fields for molecular fluids using explicit water
	Saúl Juan Carlos Salazar Samaniego	BUAP	Interaction information in threéparticle quantum systems and synergic effects
12th in 2022	José Luis Godínez Pastor	BUAP	Orientational aspects of boron nitride nanotubes in water
	Christopher Aldahir Martínez López	UG	Understanding the Aluminum ion adsorption from anodizing wastewater on hydroxyapatite using Molecular Dynamic Simulation
	Oscar Olvera Neria	UAM-Azcapotzalco	Structure prediction of insulin with mutations using AlphaFold
13th in 2023	Luis A. Castillo-Félix	ITC	Theorethical-experimental study of the rheological behavior of the ionic liquid 1-butyl-2,3-dimethylimidazolium tetrafluroborate
	Sofía del Carmen Torres Revuelta	IIM-UNAM	Stability study of phospholipid vesicles, DPPC, with cholesterol for the transport of an insulin monomer: zeta potential and interactions of amino acid residues with the polar heads of phospholipids, a study with molecular dynamics
	Ana Beatriz Salazar Arriaga	IIM-UNAM	*Aplicación de campos eléctricos en la fisicoquímica de la desorción de una mezcla de hidrocarburos y tensoactivos: Dodecilsulfato de sodio (SDS), sobre grafito: un estudio por dinámica molecular*

Fig. 5. Winners of the Poster session in the 7th Meeting on Molecular Simulations in 2015. From left to right. Alexander Pérez de la Luz (UAM-Iztapalapa), Patricia Morales de Tirado (JCTC), Julian Tirado-Rives (Yale University, USA), Sandra Guadalupe Hernández Ríos (UASLP) and Janett Torres Ruíz (IPN). All of the winners were awarded with a prize of $250 usd provided by the Journal of Chemical Theory and Computation.

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

The Meeting is organized in two and half days. The number of conferences is around 15 given by around 4 researchers from other countries, 7 consolidated Mexicans **researchers** and 4 graduate/postdocs participants. The guests speakers have come from different countries such as: United States, Spain, England, Germany, Ukraine, Portugal, Canada, Peru and Chile.

The information of the Meetings can be found in the web page https://www.dci.ugto.mx/~molsim. In Fig. 6 attendees to the 7th Molecular Simulation Meeting in 2015 are **shown**.

Fig. 6. Participants at the 7th Molecular Simulation Meeting in 2015. The photo was taken in front of the Cathedral in the Zócalo of Mexico City.

Professor José Alejandre was the organizer of the first Meeting on Molecular Simulations in 2009, since then, he has been member of all the Meetings celebrated anually until 2023. The year 2021 y 2022 the Meeting was cancelled because the COVID pandemic. The number of organizers has increased with time. In 2024, the Meeting is being organized by Professors Jorge López-Lemus (UAEMex), Edgar Núñez-Rojas (CONAHCyT-UAM), Omar Castrejón (ITC), Héctor Domínguez-Castro (UNAM), Cesar Millán-Pacheco (UAEM), Susana Figueroa Gerstenmaier (UG), Alexander Pérez de la Luz (UAM), Francisco Alarcón Oseguera (UG) and José Alejandre (UAM). See also Fig. 7. The members of the Organizing Committee in previous years can be found in web page https://www.dci.ugto.mx/~molsim.

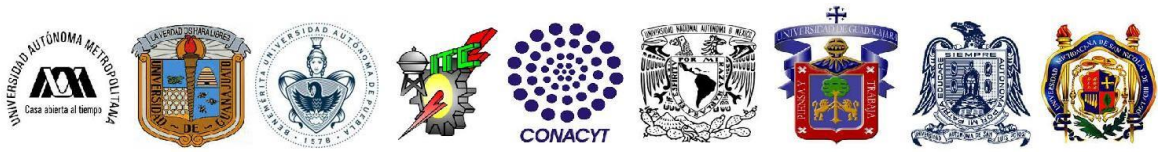

Fig.7. The institutions where the Organizing Committee work for.

Molecular Simulation prize. Being part of a community

The Selection Committee to evaluate the proposals of the simulation community to award the prize to a researcher for the next Meeting are the last three winners of the simulation prize. The prize is awarded every two years during the Meeting to a national researcher whose research area is molecular simulation and who has made relevant scientific contributions in that field. The training of students and the promotion of molecular simulation in Mexico and abroad are also considered. The Prize consists of a diploma given during the special dinner of the event.

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Prizes have been awarded to UAM-Iztapalapa researchers: Professors Gustavo A. Chapela in 2010, Fernando del Río in 2012 and José Alejandre in 2014. Professor Alejandro Gil-Villegas from *Universidad de Guanajuato*, Campus Leon, was awarded in 2016. In 2018 the prize was received by Professor Héctor Domínguez from UNAM and finally, the last prize was awarded to Professor Ramón Castañeda Priego from *Universidad de Guanajuato* , Campus Leon, in 2022. In 2020 there was not prize because the Meeting was not organized due to the Covid pandemic. Fig. 8 shows the winners of Molecular Simulation Prize.

Fig. 8. Winners of the prize of the Molecular Simulation Meetings. From lef to right: Professors José Alejandre, Gustavo A. Chapela, Fernando del Río, Héctor Domínguez, Ramón Castañeda and Alejandro Gil-Villegas. Picture was taken during the 12th Meeting organized in the hotel NH in the center of México City (2022).

Funding. Paying is not a simulation

The Meetings have been organized thanks to the high interest of the Organizing Committee. Sometimes they have to pay their own expenses and also those of their students. The *División de Ciencias Básicas e Ingeniería* from UAM-Iztapalapa has given us financial support for all the Meetings. The support has been used to pay accommodation and transportation for some students and invited speakers. In some cases, the *Rectoría* of UAM-Iztapalapa and *Rectoría General* have also supported us. In years 2012, 2013, 2014 and 2018 CONAHCyT approved financial support to organize the corresponding *Meeting on Molecular Simulations*. It was possible to pay accommodation and transportation for most of students and invited speakers. The number of participants grew significantly during those years. In the last three meetings we have been forced to charge a registration fee to recover part of the expenses.

In general, in Mexico, university academic programs do not include mandatory molecular simulation courses. In some of them, the students can take optional courses given by their thesis director in most of the cases. That is one of the reasons why the organization of these Meetings is important. The students and researchers have the opportunity of knowing the state of the art research that is being doing in this field. The financial support allows to increase the number of participants.

National workshops on Molecular Dynamics

Professor Alejandre has always been concerned in providing students with updated information on the methodologies to undertake scientific investigation either on the theoretical basis of the molecular modeling and simulation techniques, the development of molecular models and computational algorithms or even their application to provide mechanistic explanations of specific physicochemical phenomena in condensed phases, in terms of the motions and interactions of the constituent molecules. This urge enticed him from the very first

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Meeting on Molecular Simulation (MMS 1, 2009), to propose that the event should encourage students not only to present their own research, but also to learn more about the topics relevant to the field; thus, a first session of the event was devoted to three two-hour lectures on (1) the foundations of calculations of electronic structure, (2) the foundations of molecular dynamics simulations and (3) a "hands-on" workshop in which the students would get to perform some actual computations of simple systems.

Whereas the first two subjects can be taught in a standard, conventional manner, the third one posed a significant challenge as it requires adequate computers, computer codes and, most importantly, some previous knowledge on "computer handling" from the students. Despite this difficulty, the proposal's success can be gauged by the enthusiastic participation of tens of students. However, it became clear that the attendees had various levels of knowledge and skills, leading to a wide variety in the benefits that they could get from the experience. It also became clear that the subjects relevant to molecular modeling and simulation were not part of any curricula in Chemistry or Physics in Mexico.

As a consequence, and at Professor Alejandre's initiative, the project of a *Taller de Dinámica Molecular* (TDM, Workshop on Molecular Dynamics) was born with the aim of grouping as many colleagues as possible, who worked on the disciplines of molecular modeling and simulation and were convinced of the necessity of sharing and extending the knowledge they got from abroad, as well as the convenience of constituting a Mexican community firmly based on preparing new generations of scientists with the ability to undertake what is now known as multi-, inter- and transdisciplinary research in molecular science, combining the traditionally separate disciplines of biology, chemistry, computational science, mathematics and physics to pursue the understanding of complex phenomena in the terms described above.

The first TDM took place from July 25th to 29th, 2011, hosted by the colleagues at *Universidad de Guanajuato* (UG), see Fig. 9, led by Professor Ana Laura Benavides who was the main organizer of the workshop. The attendees were mainly the students of the instructors who lectured at that time. It is worth to mention that each lecturer and each attendee covered his own expenses regarding housing and food. While UG provided the halls, general logistics and coffee, cookies were a generous contribution from Professor Benavides. Each attendee was asked to bring along his own computer. Each instructor provided the programs and input data files required for his lecture by means of a memory key. All the software used in the workshops has been Open-Source code. The attendees were distributed in three groups according to their own appreciation of their level: beginners (B), intermediate (I) and advanced (A).

The TDM was hosted by UG until 2013, then moved to Cuernavaca where Professor César Millán, from *Facultad de Farmacia* at *Universidad Autónoma del Estado de Morelos* (UAEM), and Professor Humberto Saint-Martin, from *Instituto de Ciencias Físicas* (ICF) at *Universidad Nacional Autónoma de México* (UNAM), undertook the organization with the help of colleagues from BUAP, UAM, UG, UNAM and *Tecnológico Nacional de México* (TecNM). Fig. 10 shows participants of the 4th TDM held at the ICF, UNAM. Younger colleagues from *Universidad de Guadalajara* are now in the Organizing Committee.

The polls that were conducted in the first six TDM's showed the need to include new topics in the Program; ever since, the subjects to be covered have been updated every year so that the TDM currently includes state of the art topics with a high demand from new communities, such as students and researchers in Biochemistry and Pharmacy. The evolution of the TDM is summarized in Table 2, from the original three groups (B), (I) and (A) to those added in 2017, when the (I) was eliminated: (Ap) applications in general physical chemistry; (P) "programmers", for attendees interested in developing force fields and algorithms, as well as in parallel programming; (BF) applications of molecular modeling and simulation to Biochemistry and Pharmacy; (QM) for those interested in classical molecular dynamics of atoms moving in the potential energy of the electrostatic repulsion between nuclei and the potential energy computed from "on-the-fly" electronic structure calculations.

It is worth to mention that the highest demand from the TDM is for the groups of beginners and of applications to biochemistry and pharmacy. More modern topics, such as *ab initio* molecular dynamics, have also been considered; courses in the use of Machine Learning techniques and the use of Artificial Intelligence will be included as of 2025.

The event was financially supported by ICF in 2014. From 2015 to 2018, additional funding was provided by the Government of the State of Morelos, through the now extinct *Secretaría de Innovación, Ciencia y Tecnología* (SICyT-Morelos), and by the Mexican Federal Government through the also now extinct Special Program to Support Scientific, Technological and Innovation Activities from *Consejo Nacional de Ciencia y*

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Tecnología (then CONACyT, now CONAHCyT). This funding is labeled as "Full" in Table 2. Fig. 11 shows participants of the 8th TDM held at the ICF, UNAM, Cuernavaca, Morelos in 2018.

The change of both the State and the Federal governments entailed the extinction of the escrows for scientific projects, thus a much more limited access to funds for all scientific activities; a solution had to be found to keep the TDM going. The Organizing Committee decided to charge a fee starting in 2019, that should cover all housing and meal expenses for the lecturers and attendees. The results vastly surpassed the expectations, to such an extent that a surplus was obtained and allowed the whole TDM to be held at the same location where the attendees were lodged. This is labeled as "Self" in Table 2.

The 10th TDM had to be delayed for one year, due to the "confinement by COVID" in 2020; it was performed online in 2021 and the invitation was successfully extended to other Spanish speaking countries, mainly in Latin America. The fee was then used for Zoom accounts and for the use of remote computing. Fig. 12 shows a snapshot of a screen with online participants during the 10th TDM in 2021. Though the number of attendees was cut down to less than 25% of the 8th and 9th TDM's, the event is still ongoing and expected to grow again.

Table 2. The twelve TDM workshops that have taken place since 2011; due to the COVID confinement, the event was not done in 2020. The asterisk (*) in the number of attendees indicates an estimate. The next TDM has the "lucky number" 13, that should result in a vigorously renewed event.

No.	Year	Dates	Place	Groups	No. Attendees	Financial support
1	2011	July 25 to July 29	Guanajuato	B, I, A		No
2	2012	August 20 to August 24	Guanajuato	B, I, A		No
3	2013	August 5 to August 9	Guanajuato	B, I, A		No
4	2014	July 28 to August 1	Cuernavaca	B, I, A	60*	ICF
5	2015	July 27 to July 31	Cuernavaca	B, I, A	80	Full
6	2016	July 25 to July 29	Cuernavaca	B, I, A	171	Full
7	2017	July 31 to August 4	Cuernavaca	B, A, Ap, P, BF	190	Full
8	2018	July 30 to August 3	Cuernavaca	B, A, Ap, P, BF	200*	Full
9	2019	July 29 to August 2	Cuernavaca	B, A, Ap, P, BF	200*	ICF+Self
*	2020	COVID			None	
10	2021	August 2 to August 6	Online	B, A, Ap, P, BF	45	Self
11	2022	August 1 to August 5	Online	B, A, Ap, P, BF, QM	61	Self
12	2023	November 20 to November 22	Hybrid	B, A, Ap, P, BF, QM	60*	Self
13	2024	June 24 to June 28	Cuernavaca	In progress		Self

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Fig. 9. Lecturers and attendees to the 1st TDM, ***Universidad de Guanajuato***, 2011.

Despite the difficulties, it is now clear that the event will keep attracting the interest of future developers and users of molecular modeling and simulation techniques. Moreover, several former alumni have volunteered to lecture on their own areas of expertise, all related to molecular sciences, and provided the TDM with a continuous renewal of topics. That is to say, the new generations are keenly aware of the relevance of the field and willing to contribute to its progress by updating not only the topics to be taught, but also how communication with colleagues is established throughout the Spanish-speaking communities, for instance, a Facebook group is already available at https://www.facebook.com/groups/144556469018023

Fig. 10. Lecturers and attendees to 4th TDM, Cuernavaca, 2014.

Fig. 11. Lecturers and attendees to 8th TDM, Cuernavaca, 2018.

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

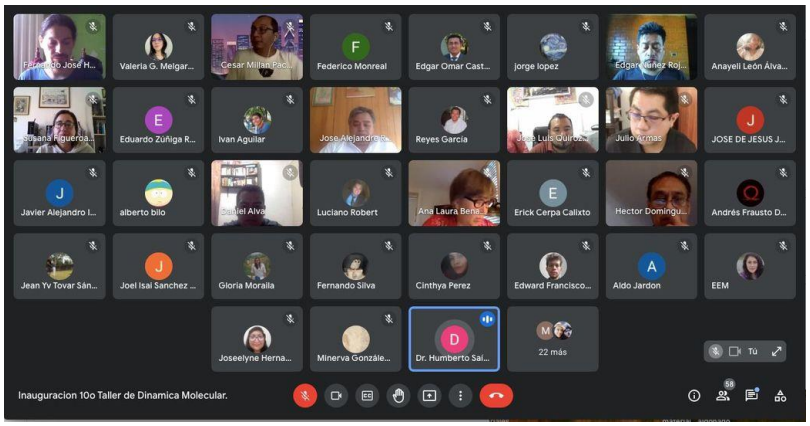

Fig. 12. Lecturers and attendees to 10th TDM, online, 2021.

Computer Simulations in the world, Mexico and at UAM

In Fig. 13 it can be observed the number of articles published in the world, in Mexico and in **UAM** organized per decades. Topics searched in the Web of Science were *Molecular Dynamics* and *Monte Carlo Simulations* [6]. In Fig., decades are defined with the initial year. It was considered as the first molecular simulation article *J. Chem. Phys. 27, 1208 (1957)* by B. J. Alder and T.E. Wainwright in 1957. It is interesting to note that throughout the world there was a great advance in molecular simulation research from 1990 to 1991 and these years coincide with the development of the LINUX operating system [7]. Also, in 1991, with Java, object-oriented programming began to be relevant in the field of computing [8] and the Gopher protocol was created at the University of Minnesota; this is an internet system that preceded the world wide web [9].

In Fig. 13 it can be seen that the production of Molecular Dynamics articles in Mexico is 1% of the world and that, in turn, the articles production of UAM is 10% of Mexico's production. In the case of Monte Carlo articles, the trend is the same, however, the production of articles about MC, in general, is lower than that of MD articles.

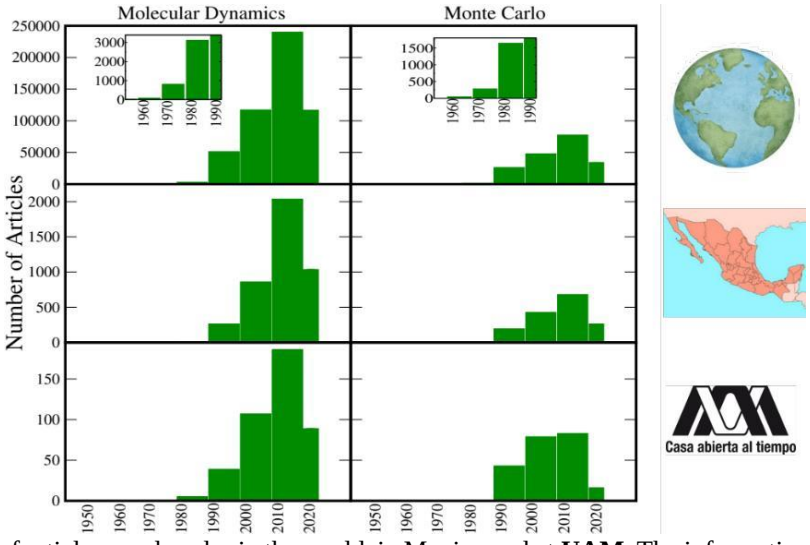

Fig. 13. Number of articles per decades in the world, in Mexico and at **UAM**. The information is extracted from Web of Science where the legends "*Molecular Dynamics*" and "*Monte Carlo simulations*" were searched.

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Molecular Dynamics and Monte Carlo simulations articles production of different countries and Mexico

In the Fig. 14 it can be observed the global production and two examples of countries that produce more than a half of the molecular dynamics articles in the world. Decades are denoted as it has been already described. These countries are the United States of America and China, which, as can be seen in the Fig., had considerable growth starting in 2011. On the other hand, the United States has been increasing its production constantly.

With a production equivalent to around 10 % of world production we have Spain, Canada and Brazil. Finally, as it has been already explained in Fig. 13, we present three countries whose production is, on average, 1 % of world production, these countries are Argentina, Chile and Mexico.

The trends in Monte Carlo articles are presented in the right panel of Fig. 14 and they are similar to those shown in the previous figure.

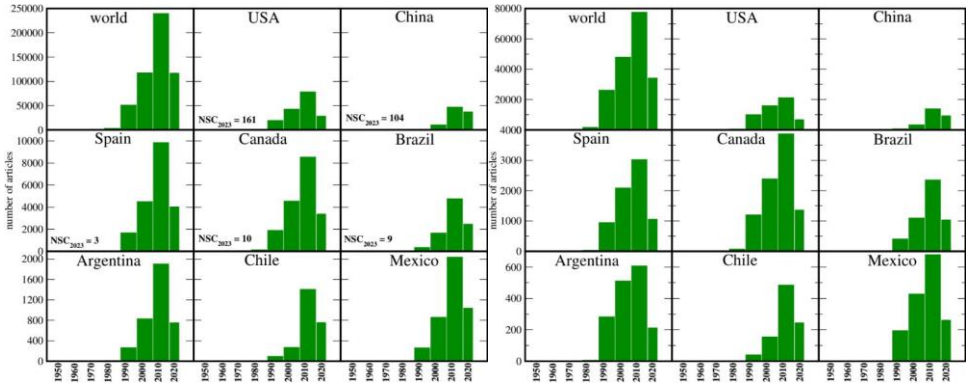

Fig. 14. Number of articles by decade in the world and different countries. The information is extracted from Web of Science where the legend *Molecular Dynamics* was searched, left panel. The *Monte Carlo* search are shown in the right panel. The number of supercomputers, NSC, within the TOP500 ranking in 2023 that every country had is shown in the figure.

Supercomputing in the world. May the power be with us

The development of computer simulations requires the use of high performance computers. How are we in Mexico compared with other countries? The TOP500 project ranks the world's fastest computers twice a year from 1993 [10]. Fig. 15-A shows countries that have high-performance computers measured in peta-FLOPS (a peta-flop means 10^{15} floating point operations per second) since November 2006. Currently, the United States has the largest number of supercomputers on the list, with 161 machines. As of November 2006, the United States had 306 supercomputers, as it was on a downward trend of machines until 2021; the decrease in the number of supercomputers and the increase in the production of simulation articles (see Figures 13 and 14) may be due to the efficient use of computational resources. The European Union is in second place with 112 machines, in recent years it has a constant trend in the number of machines, but as of 2021 it shows an increase in the number of machines. China is in third place with 104 machines, but in 2006 it only had 18 and in 2010 it had 228 machines. As of 2020, China has had a decrease in the number of machines. Countries such as: Canada, Brazil and Spain have a smaller number of high-performance machines than the US and China. While Mexico practically does not have a high-performance machine since 2017, see Fig. 15-B. In 2007 China had 9 supercomputers in the rank TOP500 in 2007 then went to around 230 in 2019, an increase of 25 times in 12 years. Finally, in 2023 they have around 100. It is probably that because the new computers are faster than the older the calculations are performed in less time. That might the same situation in USA. Although Argentina and Chile do not have a significant presence in the number of supercomputers in the world, their production of simulation work is comparable to that of Mexico (see Figures 13 and 14). By analyzing articles

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

from 2022 and 2023, it can be seen that this advance in production may be due to collaborations with research groups from other countries such as France, Germany, USA and India.

In Mexico we have the *Delta Metropolitana de Cómputo de Alto Rendimiento* formed by UNAM, UAM and CINVESTAV (IPN). The idea was to connect the computers of the three institutions, but for some reason it is not working. It seems that even putting together the three computer the TOP500 ranking is not reached. The information provided in this work is useful to understand how is the supercomputing development in Mexico. Without powerful computers not only the molecular simulation community is affected but also other areas of knowledge as electronic structure, astronomy, etc.

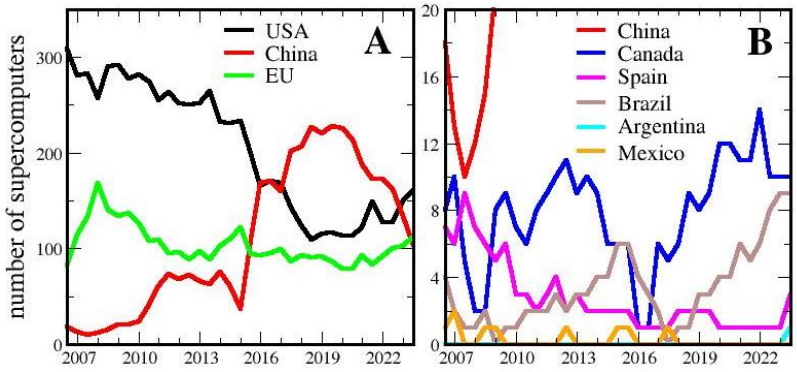

Fig. 15. Number of supercomputers in several countries as a function of time. **(A)** USA, China and Europe. **(B)** China, Canada, Spain, Brazil, Argentina and Mexico.

Molecular Dynamics and Monte Carlo simulations in Mexico

In Fig. 16 the distribution of molecular dynamics articles production is presented for decades indicated in Mexico. It is interesting to observe that in the first decade (1984-1993) in Mexico there were only seven institutions performing Molecular Dynamics simulations. Also, from 1984 to 2003 UNAM published most of the half articles of the molecular simulations field; on this period, UAM was in second place publishing molecular dynamics articles. In the decade 1994-2003 several institutions began to work in the field, mainly UG, UAEM, UANL**, UASLP** and UMSNH. These institutions have had presence in the las three decades. Also, from 2004 IPN started to increase its production. From 1994 to 2013 the IMP made an important contribution to the production of molecular dynamics articles, however, from 2013 to 2024 this contribution decreased significantly.

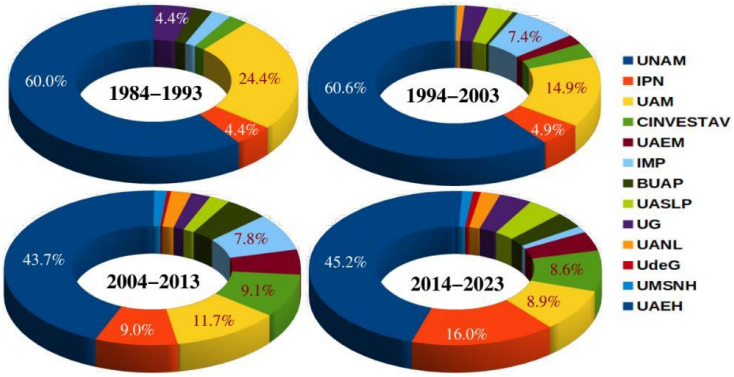

Fig. 16. Distribution of the articles production of different Mexican institutions. The search was *Molecular Dynamics* in the Web of Science. The results are given periods of ten years. The number of articles per decade is: (45:1984 to 1993), (350:1994 to 2003:), (940:2004 to 2013) and (2037:2013-2023). The total number of articles is 3372.

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

In Fig. 17 the distribution of Monte Carlo simulations articles production is presented for decades indicated in Mexico. In the decade from 1984 to 1993 there were only five institutions publishing articles on this topic, UNAM, IPN, UAM, CINVESTAV and UASLP. From 1994 IMP, UG, UAEM and BUAP started to work and publish on this direction.

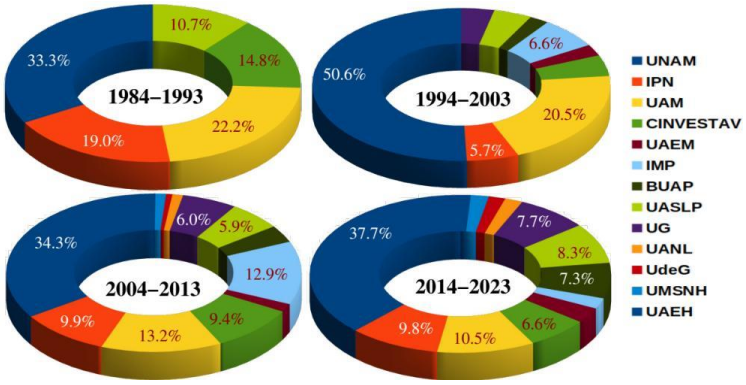

Fig. 17. Distribution of the articles production of different Mexican institutions. The search was *Monte Carlo simulations* in the Web of Science. (27: 1984 to 1993), (336:1994 to 2003), (597; 2004 to 2013) and (726: 2013 to 2023). The total number is 1686.

Most cited articles of the Mexican molecular simulations community

A list of articles in molecular simulation field by at least one Mexican author with more than 100 citations is presented in Table 3.

The molecular simulation community is still in its development stage. The first articles published in international journals in this area were developed in the 1980s. It is a relatively new subject. To evaluate the impact of the Mexican community in this field we decided to look for the articles with WofS citations greater than 100. The names of the Group leader in bold face letter, the number of citations, reference and doi for every of the highlighted papers are given in Table 3. A chronological analysis by topics is made with the following arbitrary classification:

1. Purely theoretical investigations that use molecular simulations to compare their description of either ideal or realistic systems, denominated as “Basic Theory” (BT) in Fig. 18.
2. Development of algorithms and programs, ranging from MD engines to analysis tools (AP).
3. Design of novel molecular models and/or parameterizations of force fields (FF).
4. Applications to novel descriptions of various physicochemical phenomena and systems (PP) and, due to its growing relevance and ongoing participation of researchers in biological sciences, a separate account was made for
5. the use of MMS in describing biomolecular systems and looking for pharmaceutical drugs (BioPh).

The main journals where articules with more than 100 citations have been published are

J. Chem. Phys (15), Phys. Rev. E (6), J. Phys. Chem. B (5), Phys. Rev. Lett (3), Molec. Phys (2) and J. Phys. A: Math. Gen (2). Surface Science (2), Chem. Review (1), Nature (1), Structure (1)

The first high-impact article dates to 1977, with the pioneering work of Professor Gustavo A. Chapela on describing a gas-liquid surface of a system of Lennard-Jones molecules through MD and Monte Carlo simulations, to provide computational and numerical support to simulations of complex systems of particles with a simple model of their interactions.

Though research in different topics was undertaken by several Mexican groups, for the first years (1977 to 1990), the most relevant was only on the use of MMS to validate basic theoretical work, as done by Professor Marcelo Lozada-Cassou, who used Monte Carlo simulations to validate several results from the **hypernetted-chain and mean-spherical integral equations**, and Professor Magdaleno Medina-Noyola, with studies of the

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

electrical double layer and **on** the diffusion of solutes through various solvents. Professor Fernando del Río has made important contributions in the development of theoretical thermodynamics for liquids.

Table 3. Group leader, first author, number of citations, references and DOI of molecular simulation articles published by Mexican researchers living in Mexico and having more than 100 citations. The DOI for article with (*) is: 10.1002/(SICI)1096-987X(19990415)20:5<511::AID-JCC4>3.0.CO;2-8. There are 32 group leaders shown in bold letters.

Group Leader	First Author	Citations	Reference	DOI
Alejandro Gil-Villegas	**Gil Villegas, A.**	**901**	**J. Chem. Phys. 106, 4168–4186 (1997)**	**https://doi.org/10.1063/1.473101**
	Amparo Galindo	347	Molecular Physics, vol. 93, Issue 2, p.241-252 (1998)	https://doi.org/10.1080/00268979809482207
	Eduardo Buenrostro-González	222	AIChE Journal; 2004 , 50, No. 10	https://doi.org/10.1002/aic.10243
	Amparo Galindo	189	J. Phys. Chem. B 1999, 103, 46, 10272–10281	https://doi.org/10.1021/jp991959f
	Clare McCabe	118	J. Phys. Chem. B 1998, 102, 41, 8060–8069	https://doi.org/10.1021/jp982331s
José Alejandre	**José Alejandre**	**601**	**J. Chem. Phys. 102, 4574–4583 (1995)**	**https://doi.org/10.1063/1.469505**
	Mark E Tuckerman	414	J. Phys. A: Math. Gen. 39 5629 (2006)	https://doi.org/10.1088/0305-4470/39/19/S18
	Andrij Trokhymchuk	407	J. Chem. Phys. 111, 8510–8523 (1999)	https://doi.org/10.1063/1.480192
	Minerva González-Melchor	149	J. Chem. Phys. 125, 224107 (2006)	https://doi.org/10.1063/1.2400223
	Pedro Orea	110	J. Chem. Phys. 123, 114702 (2005)	https://doi.org/10.1063/1.2018640
	Raúl Fuentes-Azcatl	102	J. Phys. Chem. B 2014, 118, 5, 1263–1272	https://doi.org/10.1021/jp410865y
Chapela, Gustavo A.	**Gustavo A. Chapela**	**353**	**J. Chem. Soc., Faraday Trans. 2, 1977,73, 1133-1144**	**https://doi.org/10.1039/f29777301133**

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Group Leader	First Author	Citations	Reference	DOI
Garzon, Ignacio L.	**I. L. Garzón**	**363**	**Phys. Rev. Lett. 81, 1600 (1998)**	**https://doi.org/10.1103/PhysRevLett.81.1600**
	K. Michaelian	329	Phys. Rev. B 60, 2000 (1999)	https://doi.org/10.1103/PhysRevB.60.2000
	Cecilia Noguez	288	Chem. Soc. Rev., 2009,38, 757-771	https://doi.org/10.1039/b800404h
	José M. Soler	170	Phys. Rev. B 61, 5771 (2000)	https://doi.org/10.1103/PhysRevB.61.5771
	Ignacio L. Garzón	117	Phys. Rev. B 54, 11796 (1996)	https://doi.org/10.1103/PhysRevB.54.11796
	J. Jellinek	101	Atoms, Molecules and Clusters 20, 239-242 (1991)	https://doi.org/10.1007/BF01543982
Perez-Aguilar, Jose Manuel	**Ge Fang**	**400**	**NATURE COMMUNICATIONS (2018) 9:129**	**https://doi.org/10.1038/s41467-017-02502-3**
	G. Glenn Gregorio	208	Nature; 547(7661): 68–73. (2017)	https://doi.org/10.1038/nature22354
	Irina Kufareva	138	Structure 22, 1120–1139, 2014	https://doi.org/10.1016/j.str.2014.06.012
	Yiming Zhao	128	Nature Communications volume 7, 11221. (2016)	https://doi.org/10.1038/ncomms11221
Ascencio, Jorge A.	**M. José Yacamán**	**381**	**J. Vac. Sci. Technol. B 19, 1091–1103 (2001)**	**https://doi.org/10.1116/1.1387089**
	H. E. Troiani	141	Nano Letters 2003, 3, 6, 751–755	https://doi.org/10.1021/nl0341640
	J. A. Ascencio	125	Surface Science 396 (1998) 349-368	https://doi.org/10.1016/S0039-6028(97)00689-4
	Ascencio J.A.	101	Surface Science 447 (2000) 73–80	https://doi.org/10.1016/S0039-6028(99)01112-7
Laura Dominguez	**Phuong H. Nguyen**	**372**	**Chem. Rev. 2021, 121, 4, 2545–2647**	**https://doi.org/10.1021/acs.chemrev.0c01122**
	Christian Frantz	150	J Cell Biol . 2008 Dec 1;183(5):865-79	https://doi.org/10.1083/jcb.200804161

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Group Leader	First Author	Citations	Reference	DOI
Galindo-Murillo, Rodrigo	**Marie Zgarbová**	**333**	**J. Chem. Theory Comput. 2015, 11, 12, 5723–5736**	**https://doi.org/10.1021/acs.jctc.5b00716**
	Rodrigo Galindo-Murillo	301	J. Chem. Theory Comput. 2016, 12, 8, 4114–4127	https://doi.org/10.1021/acs.jctc.6b00186
	Rodrigo Galindo-Murillo	134	Nucleic Acids Research, 43, 11,2015, 5364–5376	https://doi.org/10.1093/nar/gkv467
	Rodrigo Galindo-Murillo	118	Biochimica et Biophysica Acta 1850 (2015) 1041–1058	https://doi.org/10.1016/j.bbagen.2014.09.007
Jose L Medina-Franco	**Sabrina Castellano**	**154**	**J. Med. Chem. 2011, 54, 21, 7663–7677**	**https://doi.org/10.1021/jm2010404**
	T Scior	142	Curr Med Chem . 2009;16(32):4297-313	https://doi.org/10.2174/092986709789578213
	Dirk Kuck	140	Bioorganic & Medicinal Chemistry; 18, 2, 2010, 822-829	https://doi.org/10.1016/j.bmc.2009.11.050
	Maykel Cruz-Monteagudo	118	Drug Discov Today . 2014;19(8):1069-80	https://doi.org/10.1016/j.drudis.2014.02.003
	Narender Singh	116	J. Chem. Inf. Model. 2009, 49, 4, 1010–1024	https://doi.org/10.1021/ci800426u
Koester, Andreas M.	**Matthias Krack**	**153**	**J. Chem. Phys. 108, 3226–3234 (1998)**	**https://doi.org/10.1063/1.475719**
Jose L Rodriguez-Lopez	**M. G. Méndez-Medrano**	**227**	**J. Phys. Chem. C 2016, 120, 9, 5143–5154**	**https://doi.org/10.1021/acs.jpcc.5b10703**
	Grégory Guisbiers	158	ACS Nano 2016, 10, 1, 188–198	https://doi.org/10.1021/acsnano.5b05755
	J. L. Rodríguez-López	127	Phys. Rev. B 67, 174413 (2003)	https://doi.org/10.1103/PhysRevB.67.174413
	F. Aguilera-Granja	100	Phys. Rev. B 66, 224410 (2002)	https://doi.org/10.1103/PhysRevB.66.224410

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Group Leader	First Author	Citations	Reference	DOI
Arturo Rojo Domínguez	**Leticia Arregui**	**227**	**Microbial Cell Factories,18, 200 (2019)**	**https://doi.org/10.1186/s12934-019-1248-0**
Marcelo Lozada-Cassou	**C Velasco-Santos**	**197**	**Nanotechnology 13 (2002) 495–498**	**https://doi.org/10.1088/0957-4484/13/4/311**
	Manuel Quesada-Pérez	192	CHEMPHYSCHEM2 003, 4, 234-248	https://doi.org/10.1002/cphc.200390040
	Marcelo Lozada-Cassou	190	J. Chem. Phys. 77, 5150–5156 (1982)	https://doi.org/10.1063/1.443691
	DOUGLAS HENDERSON	161	Journal of Colloid and Interface Science, 114, 1, 1986	https://doi.org/10.1016/0021-9797(86)90250-X
	Enrique Gonzales-Tovar	149	J. Chem. Phys. 83, 361–372 (1985)	https://doi.org/10.1063/1.449779
	Markus Deserno	119	J. Phys. Chem. B 2001, 105, 44, 10983–10991	https://doi.org/10.1021/jp010861+
Medina-Noyola, M.	**M. Medina-Noyola**	**195**	**Phys. Rev. Lett. 60, 2705 (1988)**	**https://doi.org/10.1103/PhysRevLett.60.2705**
	Magdaleno Medina-Noyola	146	J. Chem. Phys. 73, 6279–6283 (1980)	https://doi.org/10.1063/1.440125
Sosa-Peinado, Alejandro	**Daniel-Adriano Silva**	**183**	**PloS Comput Biol 7(5): e1002054. (2011)**	**https://doi.org/10.1371/journal.pcbi.1002054**
Jose L Rivera	**José L. Rivera**	**177**	**Nano Letters 2003, 3, 8, 1001–1005**	**https://doi.org/10.1021/nl034171o**
	José L. Rivera	152	Phys. Rev. E 67, 011603 (2003)	https://doi.org/10.1103/PhysRevE.67.011603
	José L Rivera	117	Nanotechnology 16 186 (2005)	https://doi.org/10.1088/0957-4484/16/2/003
	D. Mckay a	114	Journal of Solid State Chemistry 181 (2008) 325–333	https://doi.org/10.1016/j.jssc.2007.12.001
Osorio-revilla guillermo	**Tzayhri Gallardo-Velázquez**	**156**	**Food Research International 42 (2009) 313–318**	**https://doi.org/10.1016/j.foodres.2008.11.010**
	Ofelia G. Meza-Márquez	117	Meat Science 86 (2010) 511–519	https://doi.org/10.1016/j.meatsci.2010.05.044

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Group Leader	First Author	Citations	Reference	DOI
José M Vásquez-Pérez	**Gerald Geudtner**	**154**	**Comput Mol Sci, 2012, 2: 548–555**	**https://doi.org/10.1002/wcms.98**
Ortega-Blake, Ivan	**Mauricio Carrillo-Tripp**	**143**	**J. Chem. Phys. 118, 7062–7073 (2003)**	**https://doi.org/10.1063/1.1559673**
	Humberto Saint-Martin	114	J. Chem. Phys. 113, 10899–10912 (2000)	https://doi.org/10.1063/1.1324711
Dominguez, Hector	**H. Dominguez**	**127**	**J. Phys. Chem. B 2000, 104, 22, 5302–5308**	**https://doi.org/10.1021/jp994479x**
Faustino Aguilera-Granja	**J.M. Montejano-Carrizales**	**122**	**NanoStructured Materials, 8, 3, 169-287,1997**	**https://doi.org/10.1016/S0965-9773(97)00168-2**
	F. Aguilera-Granja	100	Phys. Rev. B 66, 224410 (2002)	https://doi.org/10.1103/PhysRevB.66.224410
Mariano Lopez de Haro	**M. López de Haro**	**125**	**J. Chem. Phys. 78, 2746–2759 (1983)**	**https://doi.org/10.1063/1.444985**
Jose-Manuel Martinez-Magadan	**J. H. Pacheco-Sánchez**	**118**	**Energy Fuels 2003, 17, 5, 1346–1355**	**https://doi.org/10.1021/ef020226i**
Santamaria, Ruben	**R. SANTAMARIA**	**116**	**J. Comput. Chem, 20, 5, 511-530 (1999)**	*
Mendoza-Huizar, Luis Humberto	**L.H. Mendoza-Huizar**	**114**	**JEAC, 521 (2002) 95–106**	**https://doi.org/10.1016/S0022-0728(02)00659-9**
Martinez-Guajardo, Gerardo	**Gerardo Martínez-Guajardo**	**111**	**Chem. Commun., 2011,47, 6242-6244**	**https://doi.org/10.1039/c1cc10821b**
	Diego Moreno	101	Chem. Commun., 2014,50, 8140-8143	https://doi.org/10.1039/c4cc02225d
Ramirez-Solis, A.	**Bernard Kirtman**	**110**	**J Chem Phys .128(11):114108 (2008)**	**https://doi.org/10.1063/1.2885051**
	Alejandro Ramírez-Solís	102	Inorg. Chem. 2004, 43, 9, 2954–2959	https://doi.org/10.1021/ic0351592

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

Group Leader	First Author	Citations	Reference	DOI
Ana Laura Benavides	**A. L. Benavides**	**107**	**J. Chem. Phys. 144, 124504 (2016)**	**https://doi.org/10.1063/1.4943780**
Jesus Muñiz	**Jesus Muñiz**	**106**	**Chem. Eur. J.2011,17, 368 – 377**	**https://doi.org/10.1002/chem.201001765**
Ramon Castaneda-Priego	**Aaron P. R. Eberle**	**137**	**Phys. Rev. Lett. 106, 105704 (2011)**	**https://doi.org/10.1103/PhysRevLett.106.105704**
	Aaron P. R. Eberle	100	Langmuir 2012, 28, 3, 1866–1878	https://doi.org/10.1021/la2035054
Fernando del Rio	**FERNANDO DEL RIO**	**103**	**MOLECULAR PHYSICS, 2002, 100, 15, 2531-2546**	**https://doi.org/10.1080/00268970210132522**
Alvarez-Ramirez, Fernando	**Fernando Alvarez-Ramírez**	**101**	**Energy Fuels 2013, 27, 4, 1791–1808**	**https://doi.org/10.1021/ef301522m**

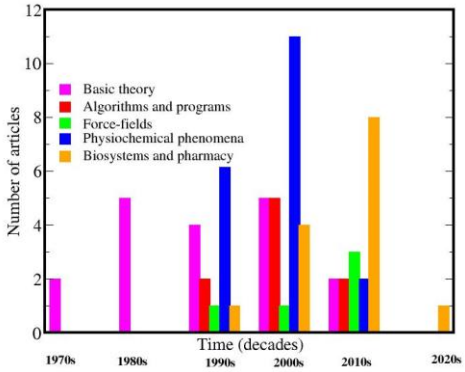

Fig. 18. Number of articles in indexed journals with more than 100 citations (WofS) as a function of time (decades) published by Mexicans researchers from the 1970s to date.

This changed in the next three decades (1991 to 2020), when molecular models, force fields and programs of Mexican origin started to be used to describe different physicochemical phenomena. Among others, it is worth mentioning the efforts by Professor Iván Ortega-Blake and his collaborators to use the interaction energies obtained from quantum calculations of electronic structure as "learning sets" to parametrize complex and sophisticated models for molecular dynamics simulations (see for instance the polarizable MCDHO water model [11]). Other lines of research to be highlighted are those of Professor José Alejandre to develop efficient codes to sample the isothermal-isobaric ensemble [12], on one hand, and to adequately consider long-range forces [13] to calculate correctly the surface tension of polar and ionic systems.

Research on biosystems and pharmaceutical drugs has become more relevant from 1991 to date, see Fig. 18, with relevant contributions by Professor Nina Pastor and Professor César Millán-Pacheco [14], as well as Professor Rodrigo Galindo-Murillo [15]. The application of molecular modeling and simulation to

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

determine properties of nanoclusters and of materials also deserves to be remarked, mentioning the contributions of Professor Ignacio Garzón, see Table 3, and of Professor Miguel José Yacamán [16].

It is important to mention that Alejandro Gil-Villegas heads the list in table 3 with the article (*Journal of Chemical Physics 106(10):4168-4186, (1997)*), he was part of the research team that developed the Statistical Associating Fluid Theory for potentials of Variable Range (SAFT-VR).

This shift to studies of bigger, more complex systems, has been possible due to access to high-performance, number-crunching computers. Unfortunately for the community, this access has been compromised in the last six years because of restricted funding from the federal government. A new strategy must be found, otherwise Mexican contributions will be severely reduced.

Leader researches in the SNI performing Molecular Dynamics simulations

In Fig. 19 the SNI level of molecular simulation professors mentioned in Table 3 is described as a distribution. Here it is possible to observe that the most of professors have a level 3 while there is a significant number of emeritus professors.

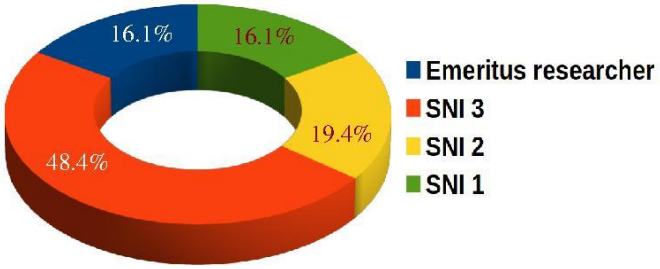

Fig. 19. Distribution of ***Sistema Nacional de Investigadores*** **(SNI)** levels in Mexican simulation research with more than 100 citations. The total number of researchers is 32.

Conclusions

Since the beginning of molecular simulations in the 1950s to date, the progress in this field of research has been notable worldwide, from the point of view of publications, in 1957 two articles on Molecular Dynamics were published while in 2023 the figure is 31296 (WofS), this, of course, is directly associated with technological advancement in computing: The United States of America, China, Germany and Japan have excellent supercomputing facilities and it is assumed that also a large number of researchers. They produce more than half of scientific articles in the world. It is interesting to see that China, in 2007 had around 10 supercomputers in the TOP500 ranking and it increased to 230 in 11 years. The number of publications increased and surely also the number of researchers. Cleary, there is a correlation between the number of supercomputers and publications in every country. More computers, more researchers, more publications and more development.

The research in molecular simulations in Mexico began around 30 years after the first molecular simulation work published in 1957. Professor Gustavo Chapela learned the methods in the United Kingdom in the 1970s and introduced them at UAM-Iztapalapa in the 1980s. Professor José Alejandre along with other Mexican researchers such as Professors Ana Laura Benavides and Humberto Saint-Martin have enthusiastically promoted the field through courses, conferences, Workshops and Meetings at the national and international level. The objectives set when the Meeting on Molecular Simulations was created have been largely met. The community collaborates in national and international projects. The number of students and postdocs in the field is growing up as it can be seen from the poster sessions of the **Meetings on Molecular Simulations**. New

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

members from different institutions are joined every year to the Organizing Committees which warrant the continuation of promoting this field in the country. The world knows the contributions made for the Mexican community in molecular simulations. The Journal of Chemical Theory and Computations has given several times economical support to award the best three poster in the Meetings. The prize of the Meeting has been awarded to 6 researchers with a high academic profile. There are around 32 leaders that have published articles with more than 100 citations (WofS) in several fields. The Journal of Molecular Liquids published a special issue with results presented in one of the Meetings. The research topics were grouped into five categories. It is shown that research is moving from the basic science, where statistical mechanics methods were used to study complex problems but with simplified models of molecular interactions, to much more complex systems in liquids, electrolytes, surfactants, polymers, ionic liquids, proteins, bilayers, etc. That trend probably is the same in other countries.

In summary, the simulation community in Mexico is developing cutting-edge research and the number of students and postdocs in the field are increasing; however, budget limitations at public universities and research facilities have resulted in the scarcity of "tenure-track positions"; moreover, as the competition for a job is open to the international scientific community, the future may look gloomy for young Mexican professional scientists; thus novel and creative solutions have to be found. The private industry supports the molecular simulation research in developed countries; more efforts have to be put on convincing both Mexican and international investors, that it is worth supporting this field through projects and the hiring of postgraduate personnel. On the other hand, we also have to join efforts with colleagues that use supercomputers for scientific research, to convince governments that investing on basic and applied science and on high-power computing facilities will be profitable. We hope that, soon, the teaching of molecular simulation methods will increase the number of mandatory courses in disciplines such as chemistry, physics, biology and different types of engineering. The fact that in the last years several professionals who work for various industries have attended the TDM gives us a moderate, but justified optimism on the future.

Acknowledgements

The authors thanks CONAHCyT for financial support provided to organize several of the Workshops and Meetings on Molecular Simulations. HSM thanks ICF-UNAM and DGAPA-UNAM for financial support, the latter through PAPIIT, grant IN109222. ENR express his gratitude to CONAHCyT for financial support under the Project *Cátedras-CONAHCyT* 687.

Summarizing the development of molecular simulations in Mexico since its appearance is a great effort that involves mentioning names, articles, workshops, courses, events and organizing committees. Throughout these years, the work of many professors, researchers and students has contributed to the advancement of this discipline, unfortunately, not all of them were mentioned in the present manuscript, let these words serve acknowledgement of their valuable contribution.

References

1. Alder, B. J.; Wainwright, T. E. *J. Chem. Phys.* **1959**, *31*, 459–466. DOI: https://doi.org/10.1063/1.1730376.
2. Barojas, J.; Levesque, D.; Quentrec, B. *Phys. Rev. A* **1973**, *7*, 1092–1105. DOI: https://doi.org/10.1103/PhysRevA.7.1092.
3. Chapela, G. A.; Saville, G.; Rowlinson, J. S. *Faraday Discuss. Chem. Soc.* **1975**, *59*, 22. DOI: https://doi.org/10.1039/dc9755900022.
4. Chapela, G. A.; Saville, G.; Thompson, S. M.; Rowlinson, J. S. *J. Chem. Soc., Faraday Trans. 2* **1977**, *73* , 1133–1144. DOI: https://doi.org/10.1039/F29777301133.

J. Mex. Chem. Soc. **2024**, *68*(4)
Special Issue

ISSN-e 2594-0317

5. Chapela, G. A.; Martínez-Casas, S. E. *Mol. Phys.* **1983**, *50*, 129–137. DOI: https://doi.org/10.1080/00268978300102221.
6. http://Quimica.Izt.Uam.Mx/Ssm/Ssm09/, accesed in 2024.
7. https://www.Britannica.Com/Technology/Linux, accessed in April 2024.
8. https://www.Britannica.Com/Technology/Object-Oriented-Programming, accessed in April 2024.
9. https://www.Chronicle.Com/Article/How-Gopher-Nearly-Won-the-Internet, accessed in April 2024.
10. https://www.Top500.Org/Lists/Top500/, accessed in April 2024.
11. Saint-Martin, H.; Hernández-Cobos, J.; Bernal-Uruchurtu, M. I.; Ortega-Blake, I.; Berendsen, H. *J. Chem. Phys.* **2000**, *113*, 10899–10912. DOI: https://doi.org/10.1063/1.1324711.
12. Tuckerman, M. E.; Alejandre, J.; López-Rendón, R.; Jochim, A. L.; Martyna, G. J. *J. Phys. A: Math. Gen.* **2006**, *39*, 5629–5651. DOI: https://doi.org/10.1088/0305-4470/39/19/S18.
13. Trokhymchuk, A.; Alejandre, J. *J. Chem. Phys.* **1999**, *111*, 8510–8523. DOI: https://doi.org/10.1063/1.480192.
14. Bencze, K. Z.; Kondapalli, K. C.; Cook, J. D.; McMahon, S.; Millán-Pacheco, C.; Pastor, N.; Stemmler, T. L. *Crit. Rev. Biochem. Mol. Biol.* **2006**, *41*, 269–291. DOI: https://doi.org/10.1080/10409230600846058.
15. Zgarbová, M.; Šponer, J.; Otyepka, M.; Cheatham, T. E.; Galindo-Murillo, R.; Jurečka, P. *J. Chem. Theory Comput.* **2015**, *11*, 5723–5736. DOI: https://doi.org/10.1021/acs.jctc.5b00716.
16. Yacamán, M. J.; Ascencio, J. A.; Liu, H. B.; Gardea-Torresdey, J. *J. Vac. Sci. Technol., B: Microelectron. Nanometer Struct.--Process., Meas., Phenom.* **2001**, *19*, 1091–1103. DOI: https://doi.org/10.1116/1.1387089.