Study of nanostructured systems for the absorption of CO2 using molecular simulation

Raul Fuentes-Azcatl[1], Héctor Domínguez Castro[1].
[1]Instituto de Investigaciones en Materiales-UNAM
Circuito Exterior, Ciudad Universitaria, Coyoacán, 04510, México, CDMX.

Global warming is one of the main concerns of our time. The anthropogenic increase of gases in the atmosphere is blamed as its main reason. Among all greenhouse gases, CO2 is the predominant one, as it causes about 60% of global warming. Reducing CO2 emissions into the atmosphere is a goal declared by governments and industry. A contribution to a global strategy is the adsorption and separation of CO2 by materials such as zeolites , activated carbon , organic metal (MOFs) , and carbon nanotubes (CNT) .

In 1997, Dillon and his colleagues first demonstrated the CNT as a potential medium for high density gas storage. Since then, CNTs have been tested to store different gases such as H2, SO2, NO2, CH4 and CO2. The main properties of the CNTs are, among others, their specific area and their adsorption sites. CNT have been considered in many works, Kowalczyk et al. used the Canonical Grand Monte Carlo technique (GCMC) to find an optimal CNT system for the adsorption of CO2 at 298 K and reported that its optimal size depends on The storage pressure. In addition, they showed that chirality does not have a strong effect on CO2 adsorption, while there is an evident dependence on the tube diameter. A similar dependence of adsorption on chirality and tube diameter for adsorption of H2 by molecular dynamics (MD). It is known that CNT lots adsorb gases better than isolated tubes, since adsorption sites are formed among CNTs, which have higher adsorption than CNT walls. Zhao et al. used the functional theory of density (DFT) to study the adsorption of various gases in single wall CNTs and packets of them.

In this work was studied the adsorption of CO2 by means of nanostructured structures. These studies will allow us to understand from an atomic-molecular point of view what are the relevant factors in the adsorption of gases by porous structures with different geometries, laminar or tubular.

Looking for BPA targets: Comparison between online docking services

Luis Martin Jiménez Rodríguez, Leonardo Daniel Olvera Aguila, Rocío Vivia Delgadillo, Rosaura Palma Orozco, Jorge Luis Rosas Trigueros

Laboratorio Transdisciplinario de Investigación en Sistemas Evolutivos, Escuela Superior de Cómputo, Instituto Politécnico Nacional, Av. Juan de Dios Bátiz s/n esq Av. Miguel Othón de Mendizabal, Lindavista, Gustavo A. Madero, 07738, Ciudad de México, México.

Human and wildlife populations are exposed to levels of BPA (Bisphenol-A) which cause adverse reproductive and developmental effects. The proteins that are targets for this molecule, as well as the molecular mechanism of the binding are not yet fully understood. In the field of molecular modeling, docking is a method which predicts the preferred orientation of one molecule to a second one to form a complex. Molecular docking has become an increasingly important tool for drug discovery as the knowledge of the preferred orientation in turn may be used to predict the strength of association or binding affinity between two molecules. This tolos can also be used to model the binding of toxic small molecules to proteins of interest. In this work we explored the interaction of BPA and candidate target proteins by means of online docking services. The results can help to better understand the adverse effects of this small molecule.

Elucidating the effect of mutations of V2 receptor in the binding of antagonists

Leonardo Daniel Olvera Aguila, Luis Martín Jiménez Rodríguez, Rosaura Palma Orozco and Jorge Luis Rosas Trigueros

Laboratorio Transdisciplinario de Investigación en Sistemas Evolutivos, Escuela Superior de Cómputo, Instituto Politécnico Nacional, Av. Juan de Dios Bátiz s/n esq Av. Miguel Othón de Mendizabal, Lindavista, Gustavo A. Madero, 07738, Ciudad de México, México

Autosomal Dominant polycystic kidney disease is a monogenetic disease characterized by renal cysts associated with pain, hypertension and a progressive loss of renal function over time. It is the fourth leading cause of end–stage renal disease (ESRD) in the United States and the most frequent inherited kidney disease.

For this work, we decided to study the antidiuretic effect of arginine vasopressin (AVP) that is mediated by the vasopressin V2 receptor, we intend, using molecular modelling, to analyse possible docking of AVP as a ligand to V2 receptor as a means to identifying important amino acid residues that might be involved in AVP binding for predicting the lowest free energy state of the protein complex. Also, we studied how selective antagonists interact differently with vasopressin V2 receptor. These findings may help design more potent and selective AVP receptor antagonists.

ALUMINATOS EN SOLUCIÓN

José Miguel Mora Fonz,[1] Gordon M. Parkinson,[2] C. Richard A. Catlow[3]
[1]Universidad Juárez Autónoma de Tabasco, DACB, A.P. 24 C.P. 86690; Cunduacán México
[2]University College London, Chemistry Department; United Kingdom
[3]Curtin University of Technology, Fuels and Energy Technology Institute, Perth, WA 6845, Australia

jmiguel.mora@ujat.mx

En este estudio hemos empleado técnicas *ab-initio* de química cuántica (Dmol^3 DFT/DNP COSMO) para modelar las estructuras de especies de aluminio monomérico en solución y su condensación para formar dímeros, tomando en cuenta las solvatación y el contraión de sodio.

Estudios previos han intentado identificar la naturaleza de las especies de aluminatos en solución.[1-3] Especies monoméricas y diméricas han sido identificadas con técnicas experimentales,[4-5] mientras otras incluyendo el trímero y tetrámero, han sido predichas.[6-7]

El estudio del proceso inicial de la condensación de especies de aluminio en solución es un problema de relevante importancia. Un campo específico donde este conocimiento es gran interés es el proceso Bayer para la extracción de aluminio a través de la precipitación de aluminatos en el cristal de gibbsita. Incrementar la velocidad de precipitación de la gibbsita es deseable para mejorar la eficiencia del proceso Bayer, donde el conocimiento de los precursores en solución es necesario.

Nuestros modelos demuestran una correlación entre el número de coordinación del aluminio con la carga del cúmulo y por lo tanto con el pH de la solución. Estos resultados además muestran la formación de un dímero estable con un doble puente (-OH-) y coordinación cinco para el aluminio, cuya formación puede ser significativa en la prenucleación de la gibbsita, ya que este doble puente es representativo de este cristal.

Referencias:
(1) Bi, S.; Wang, C. Y.; Cao, Q.; Zhang, C. H. Studies on the mechanism of hydrolysis and polymerization of aluminum salts in aqueous solution: correlations between the Core-links model and Cage-like Keggin-Al13 model. *Coord. Chem. Rev.* **2004**, 248, 441–455.
(2) Sipos, P. The structure of Al(III) in strongly alkaline aluminate solutions A review. *J. Mol. Liq.* **2009**, 146, 1–14.
(3) Zhang, J.; Klasky, M.; Letellier, B. The aluminum chemistry and corrosion in alkaline solutions. *J. Nucl. Mater.* **2009**, 384, 175–189.
(4) Buchner, R.; Sipos, P.; Hefter, G.; May, P. M. Dielectric Relaxation of Concentrated Alkaline Aluminate Solutions. *J. Phys. Chem. A* **2002**, 106, 6527–6532.
(5) Sipos, P.; May, P. M.; Hefter, G. Quantitative determination of an aluminate dimer in concentrated alkaline aluminate solutions by Raman spectroscopy. *Dalton Trans.* **2006**, 1858–1866.
(6) Gerson, A. R.; Ralston, J.; Smart, R. S. C. An investigation of the mechanism of gibbsite nucleation using molecular modelling. *Colloids Surf., A* **1996**, 110, 105–117.

Molecular Thermodynamics of Quantum Fluids using a Thermodynamic Path-Integral Perturbation Theory.

Sergio Contreras, César Serna & Alejandro Gil-Villegas
División de Ciencias e Ingenierías
Campus León de la Universidad de Guanajuato
elchaplin.sc@gmail.com, serna@física.ugto.mx,gil@fisica.ugto.mx

   We present a thermodynamic perturbation theory for fluids composed of N quantum particles with mass *m* at temperature *T* contained within a volume *V* . Our approach is based on the exact analogy between the discretized path-integral formalism of quantum mechanics and the partition function of a classical system composed of necklace molecules, introducing a Zwanzig expansion method using a quantum hard-spheres fluid (QHS) as reference system. In this way perturbation terms of the Helmholtz free energy are provided. Two different pair potentials have been considered: a) square-well (SW) and b) Lennard-Jones. In the last case we have found that it is possible to reproduce the quantum LJ fluid properties using the classical SAFT equation of state of a Mie *n-6* potential, where *n* results to be dependent of the thermal de Broglie wave-length.

Simulación molecular de cocristales metformina-cofórmero

Héctor Eduardo Jardon Valadez [1]

Departamento de Recursos de la Tierra. Universidad Autónoma Metropolitana. Av de las Garsas 10. Col El Panteón, Lerma de Villada, Estado de Mexico 52005, Mexico

En este proyecto de investigación proponemos un estudio que integra aspectos experimentales y teórico-computacionales. La mayor parte del trabajo experimental se hace de manera empírica y la obtención de nuevos compuestos es lento y costoso. Los métodos de simulación molecular son una herramienta poderosa que permite obtener información de propiedades macroscópica a partir de las interacciones moleculares de los constituyentes del sistema. Es nuestro interés aplicar esta metodología para predecir la formación y estabilidad de cocristales de interés farmacológico, así como su solubilidad en solvente orgánicos con diferente polaridad. Un cocristal se forma con moléculas que interacionan con puentes de hidrógeno. Serán estudiados cocristales del tipo fármaco-coformador y fármaco-fármaco. En particular, fármacos utilizados en el tratamiento de diabetes mellitus tipo 2, en cuadros de síndrome metabólico, obesidad y sobrepeso, como la metformina. A partir de las interacciones moleculares que estabilizan el arreglo del co-cristal, la propuesta es desarrollar nuevas formulaciones tanto de cocristales como de disolventes con mejores propiedades fisicoquímicas y/o farmacológicas.

LATERAL HETEROGENEITY IN SPHINGOMYELIN-CONTAINING LIPID BILAYERS: A MOLECULAR DYNAMICS STUDY

Fernando Favela-Rosales[1], Jorge Hernández-Cobos[2] and Iván Ortega-Blake[2]
[1]Instituto Tecnológico Superior Zacatecas Occidente
[2]Instituto de Ciencias Físicas
Universidad Nacional Autónoma de México

For decades, the cell membrane was considered as a two-dimensional lipid "sea" where integral proteins diffuse freely and laterally unless their movements were restricted by associations with other cellular components. Evidence that lipids could laterally segregate in membranes and form domains under certain conditions started to emerge back in the 1970s. These ideas did not receive much attention until the "raft" hypothesis was postulated in 1997 [1]. This hypothesis suggested the existence of domains enriched in sphingolipids and cholesterol that would be associated with specific proteins involved in cellular functions such as cell signaling and intracellular lipid traffic.

The mixtures designed to mimic putative coexisting raft and non-raft domains are usually composed of ternary mixtures of unsaturated phospholipids, Sphingomyelin and Cholesterol. To investigate the lateral structure of the rafts, molecular dynamics (MD) simulations of two points in the phase diagram determined experimentally were performed using the SLIPIDS Force Field [2]. We observed structures that support the idea of lipid rafts are present in this ternary mixture.

References:
[1] Simons, K., & Ikonen, E. (1997). Functional rafts in cell membranes. *nature*, *387*(6633), 569-572.
[2] Jämbeck, J. P., & Lyubartsev, A. P. (2012). Derivation and systematic validation of a refined all-atom force field for phosphatidylcholine lipids. *The journal of physical chemistry B*, *116*(10), 3164-3179.

Molecular dynamics simulations of sulfonated polymers

M. R. Eustaquio-Armenta[1] , M. González-Melchor[1]

1 Benemérita Universidad Autónoma de Puebla, Instituto de Física "Ing. Luis Rivera Terrazas", Apdo. Postal J-48, Puebla. Pue. C.P. 72570

Charged polymers or polyelectrolytes are used in residual water treatment and as electrolyte materials for electrochemical energy conversion and storage systems in alkaline ion and redox-flow batteries. We study sulfonated polyelectrolytes in water using molecular dynamics simulations. All atoms are included in the description. The radial distribution function, the diffusion coefficients and the radius of gyration of the polyelectrolyte are obtained using the canonical ensemble at 300 K. We also studied the conformation of the polyelectrolyte in liquid/vapor conditions.

LIQUID-VAPOR COEXISTENCE AND THE LAW OF CORRESPONDING STATES

Noemi Ochoa Mejía and Minerva González Melchor

Benemérita Universidad Autónoma de Puebla, Instituto de Física "Ing. Luis Rivera Terrazas",
Apdo. Postal J-48, Puebla, Pue. C.P. 72570
E-mail: noemi8a@gmail.com, minerva@ifuap.buap.mx

Abstract

The Van der Waals (VdW) equation of state derived in his doctoral work in 1873 exhibits coexistence of liquid and vapor phases and has a critical point. Despite the limitations that the VdW theory might exhibit, an outstanding feature is that conveniently written it takes a universal form. In 1945 Guggenheim found that the experimental liquid-vapor coexistence of different fluids collapse into a master curve. The main goal of our study is about the correspondence of states between two and three dimensions using the Lennard-Jones potential model. We use molecular dynamics to calculate the liquid-vapor coexistence curve of the two-dimensional model and estimate its critical point. With the aid of the reported data for the three-dimensional model, we explore the correspondence between two and three dimensions. We find that when the critical exponent is that of the 2D Ising model, the data do not follow the principle of corresponding states. However, by increasing the critical exponent to a certain value, the analysis suggests a correspondence of states. Finally we investigated the correspondence in terms of the cut-off radius for the two-dimensional case and we find that the liquid-vapor coexistence curves collapse to the same curve.

Perovskite bidimensional nanostructured systems for spintronics

Elizabeth Pérez-Tejada[1], Margarita C. Crisóstomo[1], Álvaro Miranda[2], Alejandro Trejo[2], Ma. Isabel Iturríos[2], Jorge Pilo[2], Eliel Carvajal[2], Rubén Vázquez-Medina[3], Miguel Cruz-Irisson[2]

[1] Instituto Politécnico Nacional, CECyT 8 Narciso Bassols. Av. de las Granjas 618, CDMX, C. P. 02530, México.
[2] ESIME-Culhuacán, Instituto Politécnico Nacional. Av. Santa Ana 1000, CDMX, C. P. 04430, México. [3]Instituto Politécnico Nacional CICATA -Querétaro. Cerro Blanco 141, Colinas del Cimatario, Querétaro, C.P. 76090, México.

Materials which exhibit half-metallic behavior are required for spintronics applications and this is the case for the Sr_2FeMoO_6 (SFMO) perovskite, at least at the bulk level; besides, many proposed spintronic devices involve thin layers. Because modifying the transition metals' relative content from the original SFMO, as well as the spatial confinement, reflects on changes of the electronic properties, for this work were modeled three insulated slabs related to the SFMO compound: the Fe:Mo ratios were 1:1, 1:0 and 0:1; the three of these slabs have free surfaces parallel to the (001) crystalline plane. All systems were geometrically optimized in the Density Functional Theory scheme, using the Hubbard corrected Local Density Approximation and the Ceperley-Alder and Perdew-Zunger functional, as implemented in the CASTEP code. Spin polarized option was employed allowing different wave functions for different spin channels. The conduction character of each insulated slab and each couple of slabs was influenced by the confinement; however, the most remarkable result is the induction of magnetic moments on the oxygen atoms [3, 4].

Key words: Spintronics, Slabs, Half-metallic, Perovskites.

References

[1] D. M. Ceperley, B. J. Alder, *Phys. Rev. Lett.***45** (1980) 566-569.
[2] J. P. Perdew, A. Zunger, *Phys. Rev. B***23** (1982) 5048-5079.
[3] J. Pilo, *et al.*, *IEEE Magnetics Letters*, 7(1) (2016) 4106403.
[3] J. Pilo, *et al.*, *J. Mol. Model.*, **23**(11) (2017) 322.

DFT study on the effects of surface passivation on the electronic properties of [110] 3C-SiC nanowires

Margarita C. Crisóstomo[1], Elizabeth Pérez-Tejada[1], M. Isabel Iturríos[1], Francisco de Santiago[2], Alejandro Trejo[2], Álvaro Miranda[2], Rubén Vázquez-Medina[3], Miguel Cruz-Irisson[2]

[1]Instituto Politécnico Nacional, CECyT 8 Narciso Bassols,. Av. de las Granjas 618, CDMX, C. P. 02530, México. [2]Instituto Politécnico Nacional, ESIME-Culhuacán, Av. Santa Ana 1000, CDMX, C. P. 04430, México. [3]Instituto Politécnico Nacional, CICATA-Querétaro, Cerro Blanco 141, Colinas del Cimatario, Querétaro, C.P. 76090, México.

Silicon carbide is an interesting material that has attracted much attention due to its properties such as chemical inertness, high hardness (9.5 mhos) and large band gap that make it suitable for applications on electronic devices operating under harsh conditions of high frequency, temperature and electrical currents. nanowires have been intensively investigated by many researchers due to their interesting properties, such as high mechanical strength, and the inherited properties from their bulk counterparts, such as chemical inertness and wide bandgap, enabling potential applications in electronics, optics, advanced engineering and nanoelectromechanical switches This work focuses on the effects of hydrogen passivation on the electronic band gap of silicon carbide nanowires (SiCNWs) grown along the [110] direction by means of Density Functional Theory and the supercell scheme [1,2]. We compare the electronic properties of fully hydrogen-passivated SiCNWs in comparison to those of SiCNWs with a mixed passivation of oxygen and hydrogen by changing some of the surface dihydrides with Si–O–Si or C–O–C bonds. The results show that, regardless of the diameter and passivation, most of the nanowires have a direct band gap which suggests an increased optical activity. The surface C–O–C bonds reduce the electronic band gap energy compared to that of the fully H-terminated phase, while the nanowires with Si–O–Si bonds have a larger band gap.

Key words: SiC nanowires, Surface Passivation, DFT.

References
[1] J. L. Cuevas, F. de Santiago, J. Ramírez, A. Trejo, Á. Miranda, L. A. Pérez, M. Cruz-Irisson, *Comput. Mater. Sci.* .**142** (2018) 268-276.
[2] M. Calvino, A. Trejo, M. C. Crisóstomo, M. I. Iturríos, E. Carvajal, M. Cruz-Irisson, *J Nanomat.***2014** (2014) 4

Electronic properties of [001] and [111] oriented diamond nanowires with nitrogen-vacancy center, a first principles study

Margarita C. Crisóstomo[1], Elizabeth Pérez-Tejada[1], M. Isabel Iturríos[1], Alejandro Trejo[2],
Álvaro Miranda[2], Eliel Carvajal[2], Marbella Calvino[2], Miguel Cruz-Irisson[2]

[1]Instituto Politécnico Nacional, CECyT 8 Narciso Bassols,. Av. de las Granjas 618, CDMX, C. P. 02530, México. [2]Instituto Politécnico Nacional, ESIME-Culhuacán, Av. Santa Ana 1000, CDMX, C. P. 04430, México.

The current tendency for modeling large molecular systems and information processing requires the development of faster and more powerful computational hardware. The physical limitations in current technologies require developments of new paradigms such as quantum computing as a crucial component for future computation and electronics. diamond and diamond nanostructures, with a substitutional nitrogen or silicon coupled with a carbon vacancy (N-V or Si-V color centers) have shown a particularly great promise for single photon emission. In this study, the electronic band structure and density of states of diamond nanowires with N-V defects were analyzed through first principles approach using the Density Functional Theory and the supercell scheme [1]. The nanowires were modeled on two growth directions [001] and [111]. All surface dangling bonds were passivated with hydrogen (H) atoms. The results show that the N-V introduces multiple trap states within the energy band gap of the diamond nanowire. The energy difference between these states is influenced by the growth direction of the nanowires, which could contribute to the emission of photons with different wavelengths.

Key words: Diamond nanowires, Nitrogen-Vacancy centers, single photon emission.

References
[1] J. Solano, A. Trejo, A. Miranda, E. Carvajal, M. Cruz-Irisson, *J. Mol. Model.***23** (2017) 292.
[2] M. Calvino, A. Trejo, M. C. Crisóstomo, M. I. Iturríos, E. Carvajal, M. Cruz-Irisson, *Theor. Chem. Acc.***135** (2016) 104

Molecular doping on halogenated silicon nanowires: An *ab-initio* study

Elizabeth Pérez-Tejada[1], Margarita C. Crisóstomo[1], Alejandro Trejo[2], Álvaro Miranda[2], Fernando Salazar[2], Eliel Carvajal[2], Marbella Calvino[2], Miguel Cruz-Irisson[2]

[1] Instituto Politécnico Nacional, C EC y T 8 Narciso Bassols. Av. de las Granjas 618, CDMX, C. P. 02530, México. [2] Instituto Politécnico Nacional, ESIME-Culhuacán. Av. Santa Ana 1000, CDMX, C. P. 04430, México.

Semiconductor nanowires are now being considered as possible basic elements for the next generation of electronic devices. Molecular doping can be a promising path to modulate their electronic properties. In general, an adsorbed molecule, added during an ex situ process, contributes with shallow electronic states inside the band gap of a host semiconductor, such as a SiNW. There are several reports on molecular doping and halogenation of nanowires [1], the combined effect of these two modifications on semiconductor nanowires has not been addressed from a theoretical point of view, to the best of our knowledge.In this work, we address the effects of molecular doping on the electronic properties of fluorinated and chlorinated silicon nanowires (SiNWs), in comparison with those corresponding to hydrogen-passivated SiNWs. Adsorption of *n*-type dopant molecules on hydrogenated and halogenated SiNWs and their chemisorption energies, formation energies and electronic band gap are studied by using density-functional-theory calculations. The results show that there are considerable charge transfers and strong covalent interactions between the dopant molecules and the SiNWs [2]. Moreover, the results show that the energy band gap of SiNWs changes due to chemical surface doping and it can be further tuned by surface passivation. We conclude that a molecular based *ex-situ* doping, where molecules are adsorbed on the surface of the SiNW, can be an alternative path to conventional doping [3].

Key words: Silicon nanowires, Density functional theory, Molecular doping, Halogens

References
[1] A. Miranda and L. A. Pérez, Electronic properties of fluorinated silicon carbide nanowires
Computational Materials Science, **111**, 294-300 (2016).
[2] A. Miranda, F. de Santiago, L.A. Pérez and M. Cruz-Irisson, Silicon nanowires as potential gas sensors: A density functional studySensors and Actuators B: Chemical, **242**, 1346-1250 (2017).
[3] F. de Santiago, A. Trejo, A. Miranda, E. Carvajal, L. A. Pérez and M. Cruz-Irisson, Band-gap engineering of halogenated silicon nanowires through molecular doping, Journalof Molecular Modeling,**23**, 314 (2017).

Monte Carlo Simulations of Self-Assembly in Quasi-One-Dimensional Systems: Soft Spheres Confined in Cylinders

Juan Germán Caltzontzin Rabell[1] José Ramón Gutiérrez Trujillo[1] Dr. Saúl Iván Hernández Hernández[2] M. en C. Nicolás Palma Aramburu[2] Dr. Abelardo Ramírez Hernández[3]

[1]Facultad de Ingeniería, Universidad Autónoma de Querétaro (UAQ), Centro Universitario, 76000 Querétaro, Qro., Mexico.

[2]Unidad Multidisciplinaria de Docencia e Investigación-Juriquilla, Facultad de Ciencias, Universidad Nacional Autónoma de México (UNAM), Juriquilla, Querétaro, CP 76230, Mexico.

[3]Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, USA.

Using Monte Carlo simulations of core-corona particles, we explore the equilibrium morphologies that arise from the interplay between the breaking of translational symmetry (due to two-dimensional confinement) and tendency of these materials to self-assembly. We found several structures as the density, size confinement and interaction range are changed. Also, we show a geometric phase-characterization procedure based on a projection of the position of center ofmass of the particles over a plane.

Monte Carlo Simulations of Self-Assembly in Quasi-One-Dimensional Systems: Soft Spheres Confined in Cylinders

Juan Germán Caltzontzin Rabell[1] José Ramón Gutiérrez Trujillo[1] Dr. Saúl Iván Hernández Hernández[2] M. en C. Nicolás Palma Aramburu[2] Dr. Abelardo Ramírez Hernández[3]

[1]Facultad de Ingeniería, Universidad Autónoma de Querétaro (UAQ), Centro Universitario, 76000 Querétaro, Qro., Mexico.
[2]Unidad Multidisciplinaria de Docencia e Investigación-Juriquilla, Facultad de Ciencias, Universidad Nacional Autónoma de México (UNAM), Juriquilla, Querétaro, CP 76230, Mexico.
[3]Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, USA.

Using Monte Carlo simulations of core-corona particles, we explore the equilibrium morphologies that arise from the interplay between the breaking of translational symmetry (due to two-dimensional confinement) and tendency of these materials to self-assembly. We found several structures as the density, size confinement and interaction range are changed. Also, we show a geometric phase-characterization procedure based on a projection of the position of center ofmass of the particles over a plane.

Detection of low-density phases of square-well parallelepipeds simulated by Event-Driven Molecular Dynamics

Anthony Bryan Gutiérrez-Romero[1] and Gustavo Adolfo Chapela[1]

[1] Departamento de Física. Universidad Autónoma Metropolitana-Iztapalapa. Av. San Rafael Atlixco No. 186, Col. Vicentina, Iztapalapa, 09340, Ciudad de México, México.

Simulations by event-driven molecular dynamics on the canonical (NVT) ensemble were performed to a variety of molecular models that consists of clusters of tangencial square-well potential spheres with a hard intramolecular potential. Each model varies as the number of spheres on their three sides changes. The initial density of the system was chosen close to the density of a possible critical density with the intention of obtaining the presence of liquid-vapor coexistence of phases by the process of spinodal decomposition, if it exists. A pattern that relates the geometry of the molecular models and the presence or absence of liquid-vapor coexistence curve was found. Radial distribution function and uniaxial order parameter was also calculated to check the presence of another phases such as crystalline and scmetic mesophase, respectively.

Molecular dynamics simulations to separate benzene from hydrocarbons using polar and ionic liquid solvents.

Edgar Núñez-Rojas[1], Hugo M. Flores-Ruiz[2] and José Alejandre[1]

[1]Conacyt-Universidad Autónoma Metropolitana-Iztapalapa. Departamento de Química. Av. San Rafael Atlixco 186, Col. Vicentina, 09340, México Distrito Federal, México.
[2]Departamento de Ciencias Naturales y Exactas, Universidad de Guadalajara campus Valles, Carretera Guadalajara-Ameca Km. 45.5, C.P. 46600, Ameca, Jalisco, México.
[1]Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa. Av. San Rafael Atlixco 186, Col. Vicentina, 09340, México Distrito Federal, México.

Molecular dynamics (MD) simulations are performed to study benzene extraction from dodecane using polar and ionic liquids solvents in a liquid/liquid equilibrium. Solvents that contain a ring structure with one and two nitrogen atoms are analyzed. Polar solvents are pyrrolidone, N-methylpyrrolidone (NMP) and pyridine while ionic solvents are 1-butyl-1-methylpirrolidonium dicyanamide [BMpyr][DCA], 1-butyl-3-methylimidazolium hexafluorophosphate [BMIM][PF6] and 1-Ethyl-3-methylimidazolium Hexafluorophos-phate [EMIM][PF6]. Results, based on density profiles analysis, show that all polar solvents studied in this work are able to absorb benzene. The [BMpyr][DCA] extracts much more benzene from the non-polar liquid than [BMIM][PF6] and [EMIM][PF6]. The [BMpyr][DCA] has slightly less affinity for benzene than the organic solvents. The partitioning of benzene between the coexisting phases was calculated.

Classical Forcefield development for the [bim-tOH][OMS] ionic liquid in Condensed Phase

Oscar Martinez-Herrrera[1], Marco Galo[1*]

[1]Tecnológico Nacional de México/ITCJ, Av. Tecnológico No. 1340, Cd. Juárez, Chihuahua, C.P. 32500, México

In this work we focus on the forcefield parametrization of the ionic liquid 1-(2- hydroxy-2-methyl-*n*-propyl)-3-*n*-butylimadazolium mesylate ([bim-*t*OH][OMs]) for applications in the area of catalysis in condensed phase.

The forcefield developed is centered on the OPLS functional, and was parameterized using a simple and robust methodology focused mainly in electrostatic charges determination and in the refinement of the most representative dihedral angles.

The calculation of the electrostatic charges followed the methodology proposed by Salas *et al.* (J. Chem. Theory Compute. 2015, 11, 683−693) involving the inclusion of polarization effects in ab-initio calculations in order to represent implicitly the solvent using the dielectric constant in conjunction with a restrain electrostatic potential fitted to an ionic liquid dimer, to account for the inclusion of solvation effects.

This forcefield parametrization methodology has been applied previously by our research group successfully for the of the [C4mim] [Oms] ionic liquid (S. Hernández-Ríos et al. Journal of Molecular Liquids 244 (2017) 422–432), and the following thermodynamic properties: densities, heat capacity, were calculated using molecular simulations in good agreement with the available experimental results.

Topological properties of hydrogen bond networks for water in different thermodynamic phases

B. V. Ramírez[1], Rosa M. Benito[2], José Torres[1], Ana L. Benavides[1]

[1]División de Ciencias e Ingenierías, Universidad de Guanajuato, León Gto., 37150, México.
[2]Grupo de Sistemas Complejos, E.T.S.I.A.A.B., Universidad Politécnica de Madrid, Madrid, 28040, España.

The study of water has always been a very active area of research among the scientific community because it is the most abundant liquid in the planet, it is fundamental for life, and it presents a very variated phase diagram. Besides, although water has a very simple molecular structure, it exhibits a great number of anomalies not found in most of simple one component fluids. These anomalies are mainly related with the formation of hydrogen bonds among molecules. So, a good water model should be able to reproduce the hydrogen bond network at different thermodynamic states. In this work we have used the Molecular Dynamics simulation technique to study the TIP4P/2005 water model at different temperature and pressure conditions to simulate single phase properties and their transitions. From the equilibrated simulated configurations we have built networks for the structure of water characterizing the hydrogen bonds with a geometrical criteria. Once the corresponding networks are well established, we computed some topological properties like the average degree, the clustering coefficient (C), the average path length (L) and the degree distributions. We noticed that the topological properties of the hydrogen bond networks are a good indicator for characterizing the distinct water thermodynamic phases (solid, liquid and vapor) and their transitions.

Study and characterization of phase transition for quasibidimensional systems

Patricia C. Tavares, A. L. Benavides, Julio C. Armas-Pérez

División de Ciencias e Ingenierías del Campus León, Universidad de
Guanajuato, CP 37150, León, Guanajuato, México

In this work we present an advance of a molecular simulation study of the Mie potential in two dimensions (disks). Four members of the Mie family potentials were selected and their liquid-vapor coexistence phase diagram together with some single state supercritical pressures and energies are presented.

Solubility of LASSBio-294 drug in different solvents using molecular dynamics

María Guadalupe Villegas González[1], Gloria Arlette Méndez-Maldonado[2] and José Guillermo Méndez-Bermúdez[3]

[1]Departamento de Fisiología y Biofísica. Universidad Autónoma de San Luis Potosí. Avenida Venustiano Carranza 2405, Los Filtros, San Luis, S.L.P.
[2]CONACYT - Departamento de Fisiología y Biofísica. Universidad Autónoma de San Luis Potosí. Avenida Venustiano Carranza 2405, Los Filtros, San Luis, S.L.P.
[3]Departamento de Ciencias Naturales y Exactas. Centro Universitario de los Valles. Universidad de Guadalajara. Carretera Guadalajara-Ameca Km. 45.5, 46600 Jal.

Cardiovascular diseases (CVD) are the leading cause of death worldwide[1]. Heart failure (HF) is a type of CVD and is characterized by a decreased ability of the heart to fill or expel sufficient blood to reach the body's metabolic needs. Currently, 3,4-methylenedioxybenzoyl-2-thienyl-hydrazone (LASSBio-294) has been synthesized as a positive inotropic prototype and alternative cardioprotector for the treatment of heart failure (HF), due to its ability to decrease the deposition of collagen at the level of the ventricles, increase exercise tolerance, improve the expression of calcium channels in the sarcoplasmic reticulum, among other benefits demonstrated in hypertensive rats with acute myocardial infarction[2].

The main problem of LASSBio-294, like many of the innovative active principles (AP), is a low solubility in water and solvents for pharmaceutical use. It is well known that the solubility of AP plays an important role in the achieved concentration of the biophase and, consequently, in the therapeutic effect[3]. For this reason, this work focuses on finding a solvent that solubilizes LASSBio-294. Specifically, We will dedicate our attention on Ionic Liquids (IL), salts which at room temperature are found in the liquid phase; they have very important characteristics, including: negligible vapor pressure, thermal and chemical stability, modifiable pH, and most importantly, their high capacity to solubilize a wide range of compounds, including AP. However, these are the same characteristics that enable them toxic[4]. In this work, the ability of [Bmim] [BF4], [Bmim] [NTF2], [Emim] [C2H3O2] and [Emim] [MeSO] to solubilize LASSBio-294 is studied using Molecular Dynamics (DM). DM is a computational simulation technique based on the resolution of Newton's equations of motion[5].

Considering that in previous studies the IL [Bmim] [MeSO] proved not to be cytotoxic, mutagenic or genotoxic against human leukocyte cells, We hereby propose it as the non toxic candidate IL to solubilize LASSBio-294[6].

[1] WHO (2015). World Health Organization. "Cardiovascular Diseases: (CVDs)". Retrieved on January 24, 2017. Website: http://www.who.int/mediacentre/factsheets/fs317/es/

[2] G. Costa, D., S da Silva, J., E. Kümmerle, A., T.Sudo, R., S. Landgraf, S., Caruso-Neves, C., A.M. Fraga, C., J. De Lacerda Barreiro, E. & Zapata-Sudo, G. (June 18, 2010). *LASSBio-294, A Compound With Inotropic and Lusitropic Activity, Decreases Cardiac Remodeling and Improves Ca 2+ Influx Into Sarcoplasmic Reticulum After Myocardial Infarction.*

[3] Resende de Azevedo, J., Letourneau, J., Espitalier, F. & Ré M. (May 27, 2014). *Solubility of a New Cardioactive Prototype Drug* in Ionic Liquids, de Journal of Chemical & Engineering data.

[4] Varneŝ, M., Tot, A., Jovanocić-Santa, S., Karaman, M., Dožic, S., Teŝanović, K., Kojić, V. & Gadžurić, S. (September 28, 2016). *Toxicity reduction of imidazolium-based ionic liquids by the oxygenation of the alkyl substituent*, de Royal Society of Chemistry.

[5] Gutiérrez, G. (April, 2001). *Elementos de simulación computacional. Dinámica Molecular y Método de Monte Carlo.* Santiago, Chile: Department of Physics, University of Santiago Chile.

[6] Gravel, J. & Schmitzer, A. R.. (December 20, 2017). *Imidazolium and benzimidazolium-containing compounds: from simple toxic salts to highly bioactive drugs.* April 28, 2017, de Royal Society of Chemistry.

Numerical simulation and experiments for wildfire behavior using symmetry plane and gravity vector approaches

Xareni Sánchez Monroy[1], José Torres Arenas[1], William Mell[2]

[1]División de Ciencias e Ingenierías. Universidad de Guanajuato. Loma del Bosque 103, Lomas del Campestre CP 37150, León, Gto., México.
[2]U.S. Forest Service. Pacific Wildland Fire Sciences Lab. 400 N 34th St., Suite 201, Seattle, WA 98103.

A simulation study was performed to improve our understanding of the slope terrain effect in wildfire propagation. Laboratory-scale experiments, which provide direct measurements of fire spread, mass loss and flame properties, as a function of terrain slope, were simulated via the Wildland-urban inteface Fire Dynamics Simulator (WFDS). WFDS is a comprehensive physics-based model in which, all the recognized coupled physical processes driving wildland fire behavior are explicitly modeled. Computational fluid dynamics (CFD) methods are used to solve numerically the three-dimensional (or two-dimensional) time-dependent equations governing fluid motion, turbulent combustion, and heat transfer.

Two approximations, made to decrease the computational cost, were tested separately. These were: the use of a vertical symmetry plane placed, span-wise, along middle of the computational domain; and modification of the gravity vector to mimic the sloped fuel bed. Comparisons between our simulations and experimental results are given.

Development of a new force field based on the criterion of Hirshfeld(charges)

Alexander Pérez de la Luz[1]; Jorge Alberto Aguilar Pineda[1]; José Guillermo Méndez Bermúdez[2]; José Alejandre[1].

[1] Departamento de Química, Universidad Autónoma Metropolitana, Iztapalapa, D.F. México.
[2] Universidad de Guadalajara, Guadalajara, Jalisco, México

In molecular simulations the force fields which contain the interaction parameters are essential for a good description of real systems. In this work is shown a methodology for the development of a new force field. In this process it was necessary to relate interaction potential parameters (charges, ε_{LJ} and σ_{LJ}) with thermodynamic properties such (dielectric constant (ε), surface tension (γ) and density (ρ)) described by Salas et al[1]. compare with various force fields, e.g. OPLS/AA[2], GAFF[3] and CHARMM[4]. In this work it is proposed to use the atomic charges obtained by the scheme of Hirshfeld[5]. This method is systematic and simple. These parameters are rescaled assuming a linear influence in properties, so that, it is possible to determine the value of the parameter which allow reproducing results close to the experimental ones. With this methodology it was obtained a force field which could be tested with temperature effects and a study of a mixture of 2 liquids.

Bibliography
1.- F. J. Salas; G. A. Méndez-Maldonado; E. Núñez-Rojas; G. E. Aguilar-Pineda; H. Domínguez and J. Alejandre; *J. Chem. Theory Comput*, **11** , 683–693, 2015.
2.- W.L. Jorgensen ; C.J. Swenson ; *J . Am. Chem. Soc*., **107**, 569-578, 1985.
3.- J. Wang; R.M. Wolf; J.W. Caldwell; P.A. Kollman; *J Comp. Chem*.; **25**, 1157-1174, 2004.
4.- B.R. Brooks; R.E. Bruccoleri; B.D. Olafson; M. Karplus.; *J Comp. Chem*, **4**, 187-217, 1984.
5. - F.L. Hirshfeld; *Theoret. Chim. Acta,* **44**, 129-138, 1977.