

Adsorción de hidrógeno en materiales porosos mediante teoría funcional de la densidad semiclásica

Susana Figueroa Gerstenmaier,^{1,} Karina Ivette Sánchez-Barroso¹, José Rubén Pérez-Mendoza¹,
Vanessa Fierro², y Alejandro Gil-Villegas¹*

¹ *División de Ciencias e Ingenierías, Universidad de Guanajuato, Campus León, México.* ² *Centre National de la Recherche Scientifique, Institut Jean Lamour, Epinal, France*

**sfigueroa@fisica.ugto.mx*

El hidrógeno ha cobrado importancia debido a su uso potencial como una de las fuentes de energía alternativa. Para poder ser usado en aplicaciones automotoras es indispensable poder almacenarlo de una manera eficiente, segura y barata. Entre las posibles opciones para resolver este problema, se encuentra la adsorción del gas en materiales porosos con una alta área superficial. El carbón activado funciona muy bien para tal objetivo, siendo además, un material abundante, accesible y que puede ser obtenido y preparado de diversas fuentes de origen vegetal, incluidos materiales de deshecho, como cáscaras de cocos, huesos de aceitunas después del prensado para obtener el aceite de oliva, etc. Cuando se preparan estos materiales porosos, dada su naturaleza amorfa y variada, es importante contar con una metodología reproducible para poder caracterizar dichos sustratos, y aún, mucho mejor, poder predecir qué tan eficaces serán para almacenar hidrógeno.

Por otro lado, la teoría funcional de la densidad (DFT) ha demostrado ser una excelente herramienta para modelar fluidos en sistemas confinados. Para ello es necesario utilizar modelos adecuados para representar, tanto el fluido como el sólido adsorbente, en combinación con información experimental. Con esto se puede, a partir de isotermas de adsorción experimental de nitrógeno a 77.4 K, y un modelo conocido como de “poros independientes”, obtener la distribución de tamaños de poros del material, y su área superficial. A partir de esta información y usando otra vez la DFT, podemos predecir la adsorción que presentará el mismo material pero esta vez para hidrógeno. Este gas, al ser un fluido cuántico, se modela de una forma más conveniente, agregando un término de corrección cuántica al potencial de interacción fluido-fluido clásico.

En este trabajo, mostramos como adicionando esta corrección cuántica, somos capaces de mejorar substancialmente el modelo clásico tradicionalmente usado para el hidrógeno en este campo. Con ello, la predicción de las isotermas de hidrógeno en carbón activado tiene una mejor concordancia con los datos experimentales.

La DFT que utilizamos está basada en la conocida como “Fundamental Measure DFT” que describe las propiedades termodinámicas y estructurales de los fluidos inhomogéneos, utilizando una aproximación de campo medio para la parte atractiva de tipo Lennard-Jones y usando un potencial de esferas duras como referencia. La corrección cuántica es introducida vía un potencial efectivo de primer orden de Wigner, con lo cual se ven modificados los parámetros del potencial Lennard-Jones (sigma y épsilon), la magnitud del diámetro de esfera dura, y la parte atractiva del potencial Lennard-Jones usada. La geometría considerada para este ejercicio es la de poros planos, por ser la más adecuada para representar al carbón activado.

Se partió de información experimental de la adsorción de nitrógeno a 77.4 K en carbono activado, junto con la descripción clásica de la adsorción, obteniendo una distribución de tamaños de poro (PSD). Por otro lado, se calcularon isotermas de adsorción de hidrógeno considerando el efecto cuántico. Finalmente, pesando las isotermas individuales de hidrógeno con esta PSD se estimó la adsorción de este gas, y se comparó con la adsorción medida experimentalmente en el mismo material.

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Estudio de Estabilidad y Reactividad Química de Confórmeros Neutros, Aniónicos y Catiónicos de Cúmulos de Al_n y $Al_{n-1}M$ ($n=3-15$; $M=Li, Na$ y K) Mediante la Teoría de los Funcionales de la Densidad

Alcántar-Medina K. O.¹; Martínez Enríquez, Arturo Isaías²

^{1,2}Centro de Investigación y de Estudios Avanzados del IPN, Av. Industria Metalúrgica 1062, Parque Industrial Saltillo-Ramos Arizpe, Ramos Arizpe, C.P 25900, Coahuila, México
e-mail: prko2009@gmail.com.

En el presente estudio, se reportan propiedades importantes acerca de la estabilidad de cúmulos neutros, aniónicos y catiónicos de Al_n y $Al_{n-1}M$ ($n=3-15$; $M=Li, Na$ o K), obteniéndose varias geometrías de confórmeros para la mayoría de las especies químicas. Se empleó la teoría de los funcionales de la densidad (DFT) con el funcional de Perdew-Burke-Ernzerhof (PBE) y un conjunto de bases triple- ζ , para calcular las optimizaciones de las geometrías mediante el programa de primeros principios Orca. Las propiedades de estabilidad que fueron calculadas son: Energía de Ionización en Adiabático (AIP), Energía de Ionización en Vertical (VIP), Afinidad Electrónica en Adiabático (AEA), Afinidad Electrónica en Vertical (VIP), Energía Homo-Lumo (Homo-Lumo gap) de sistemas Neutros y sus iones, Energía de Fragmentación (FE), Energía de Enlace (BE), Análisis de Población de Cargas de Mulliken (MCPA) para el Li, Na y K en los cúmulos, Mapeos de Orbitales Moleculares HOMO y LUMO, así como la Densidad Electrónica (ED) y la Función de Localización Electrónica (ELF). Obteniéndose criterios de reactividad y estabilidad de dichos sistemas con el objetivo de hacer predicciones acerca de cuales moléculas pueden ser empleadas en almacenamiento de hidrógeno y captación de dióxido de carbono.

Ferrofluids' diffusion dynamics and their microstructure

Ricardo Peredo Ortiz
rperedo@fis.cinvestav.mx

A ferrofluid is composed by a colloidal suspension of magnetic material (with permanent magnetic moment) in a solvent. In this work, we present results obtained from Brownian dynamics simulations, supposing that the magnetic particles interact by the Lennard-Jones potential and by the dipole-dipole potential. Furthermore, we present the system's viscoelastic modulus as a function of shear frequency, this from generalized Langevin equation and Mason's approximation for complex fluids.

DFT Study of Effect of S, P, and N in the Cationic Head of Ionic Liquids on the Interaction with Asphaltenes.

Raiza Hernández Bravo, Alma Delia Miranda, and José Manuel Domínguez

Dirección de Investigación en Exploración y Producción. Instituto Mexicano del Petróleo, Eje Central
Lázaro Cárdenas Norte 152, Colonia San Bartolo Atepehuacan, México DF. México

Using Density Functional Theory (DFT), we studied the effect of S, P, and N in the cationic head of ionic liquids, in order to study the effect of these heteroatoms in the dispersive ability of ionic liquids in asphaltenes that was done using methodologies as HOMO-LUMO interactions, electrostatic potential and Fukui reactivity Descriptors¹. This work serves as a tool to illuminate the behavior of adsorbed ions at an atomistic level. Ultimately, it is our aim that the approach taken here be extended to enable an elucidation of the parameters responsible for efficient large-scale production of stable colloidal suspensions of asphaltenes analogs in ionic liquids as asphaltenes dispersants solvents.

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Theoretical study of the quantum-chemical behavior of molecules involved in Alzheimer, Parkinson and Glioma.

Ezra Michelet García Romero ezragr_2010@hotmail.com

Cancer and neurodegeneration are usually considered opposing pathologies, the first one known for its prolonged survival and the second one for a premature cell death. Epidemiological data and molecular data using microarrays, along with *in vitro* and *in vivo* experiments seem to further contribute to this idea. This holds true especially for Alzheimer's (AD) and Parkinson's disease (PD). The relationship could be further observed using Quantum Information Theory (QIT). Information theory has been employed in neurosciences to contrast experimental data and predictive models on a regular basis and since 2005 there is an increasing interest in QIT to electronic structures revealing chemically relevant regions not shown in energy profiles. Between DNA, RNA and proteins, the latter had been chosen because of their key involvement in the diseases' pathology. Within proteins there are minimal regions known to be implicated in AD, PD and glioma pathology. Density Functional Theory serves for catalytical, pharmacological and function studies and will be taken into account for this study. The objective is to perform a theoretical study of the quantum-chemical behavior of molecules involved in PD, AD and glioma. The expected results are that molecules that converge in their pathways will have similar quantum-chemical behavior. For methodology we used Cytoscape, KEGG database, microarrays databases and research articles to find relevant pathways. After that we compiled structures from Protein Data Bank, followed by specific regions thought to contribute to these diseases. Use of different set basis (HF 6-31+G**) for electronic structure using PDB structures along with B3LYP for hardness, softness, ionization potential and electrofilicity index. And finally Shannon entropy study, Fisher Information and complexity calculations.

NOTE: RESULTS WILL BE GIVEN ON THE DAY OF THE POSTER PRESENTATION.

Diffusion coefficient of ions in two dimensions

M. R. Eustaquio-Armenta, M. González-Melchor

Instituto de Física “Luis Rivera Terrazas”, BUAP, Apdo. Postal J-48, Puebla, Pue. C.P. 72570.

The knowledge of the diffusion coefficient is indispensable to chemical engineering design and research. Molecular dynamics simulations are performed to calculate the diffusion coefficient of ions in two dimensional soft primitive model mixtures. Positive ions have charge $Z_+|e|$ and the counterions have charge fixed at $-|e|$ in the mixture. The diffusion coefficient is obtained through the velocity autocorrelation function (VACF) and the mean square displacement (MSD) as well. Good agreement between the values obtained by the two methods is found.

SHEAR FLOW OF POLYMER NANOCOMPOSITES VIA NON EQUILIBRIUM MOLECULAR DYNAMICS SIMULATION

Carrasquedo Peñaloza Carlos Arturo¹⁻², Manero Brito Octavio², Castillo Tejas Jorge³, Aguayo Vallejo Juan Pablo⁴

¹ Instituto de Investigaciones en Materiales. Universidad Nacional Autónoma de México.

² Facultad de Química. Universidad Nacional Autónoma de México.

³ Facultad de Ciencias Básicas, Ingeniería y Tecnología. Universidad Autónoma de Tlaxcala.

⁴ Centro de Ciencias Aplicadas y Desarrollo tecnológico. Universidad Nacional Autónoma de México.

Polymer nanocomposites are interesting and advanced materials due the inherent properties owing large exposed area of the reinforcement then polymer matrix. Meanwhile, molecular dynamics simulation is a powerful tool to investigate the response of macroscopic properties from molecular levels. In that sense, we use such technique to studying rheological and statics properties varying conditions of the system.

It is well know that in polymer nanocomposites, the properties are function of different variables, such as, nanoparticles dispersion, concentration of the reinforcement, level of energetic interaction, among others. Nevertheless, it has been demonstrated that the spatial organization of the nanoparticles in polymer matrix and the amount of them in the system, are the most critical variables to come a disable material. Therefore, we use equilibrium and non-equilibrium molecular dynamics simulation to analyze the response of the last conditions, to statics and dynamics properties. The simulations were carried out using Lennard-Jones (1) potential

$$U_{LJ}(r_{ij}) = 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] - U(r_c) \quad (1)$$

to represents polymer beads and polymer-nanoparticle interaction, and FENE potential (2), to represents the bonds of the polymer beads

$$U_{FENE}(r_{ij}) = -\frac{k_v R_o^2}{2} \ln \left[1 - \left(\frac{r_{ij}}{R_o} \right)^2 \right] \quad (2)$$

equations that are related to coarse grained simulations.

PROPUESTA DE MODELO POLARIZABLE PARA ALCOHOLES PRIMARIOS BASADO EN LA POLARIZABILIDAD DEL GRUPO HIDROXILO

Manuel Martínez Jiménez,^{1,2} Humberto Saint-Martin Posada²

¹Posgrado en Ciencias Físicas, UNAM

²Instituto de Ciencias Físicas, UNAM

mm_ximenez@yahoo.com

Se presenta la propuesta de un modelo polarizable de tipo densidades de carga móviles con osciladores armónicos (MCDHO por sus siglas en inglés) para alcoholes primarios, a partir de los resultados obtenidos mediante cálculos ab-initio para caracterizar las propiedades geométricas y electrostáticas de los monómeros de metanol, etanol y propanol. En los cálculos ab-initio se empleó el método MP2 para el tratamiento de la correlación electrónica y las bases aug-cc-PVxZ (x=D, T, Q y 5), con el objetivo de caracterizar el límite del conjunto base completo (CBSL por sus siglas en inglés).

Mario Raymundo Hernandez raymundo.92@hotmail.com

Estudios realizados in vitro en homogenados de corteza renal expuestos a plomo, han indicado que la actividad de la enzima GST se ve inhibida en presencia de concentración creciente del metal en función del tiempo de exposición, los resultados demuestran que la actividad enzimática se ve influenciada directamente por la presencia del metal, por lo anterior y debido al significado biológico que esta enzima tiene se realizó una dinámica molecular, en la cual se simuló primero el GSH (glutathione) reducido con la enzima Glutathione S-Transferase el cual los primeros resultados fueron satisfactorios ya que nos dieron los primeros sitios de interacción entre el ligando con la enzima GST el cual nos ayudara en las próximas investigaciones para proponerla como posible biomarcador de toxicidad de plomo, estos estudios también nos están ayudando para determinar cual es la especificidad de esta enzima.

Conformational Dynamics of the RmlA Enzyme along the Biosynthesis Pathway of dTTP-L-rhamnose. Exploring an Allosteric Enzyme Regulation Mechanism.

Héctor Eduardo Jardón-Valadez h.jardon@correo.ler.uam.mx

L-rhamnose is a 6-deoxyhexose that forms a diverse kind of glycoconjugates in the cell wall of pathogenic bacteria. dTDP-L-rhamnose is a precursor of the L-rhamnose, and it is synthesized from the nucleotide deoxy-thymidine-triphosphate (dTTP) and glucose-1-phosphate (G1P) by a four-step reaction sequence involving enzymes highly conserved in bacteria and absent in humans. The Glucose-1-phosphate thymidyltransferase (RmlA) enzyme catalyzes the first reaction of the dTDP-L-rhamnose biosynthesis, the condensation of thymidine triphosphate and glucose-1-phosphate to produce dTDP-D-glucose, and its crystallographic structure has been elucidated at high resolution (1.66 Å). In this work we generated molecular dynamics trajectories, using high performance computing resources, to analyze the conformational dynamics of the RmlA enzyme in solution, and complexed with dTTP and/or G1P. We set up four systems and prolonged the simulation trajectories up to 100 ns each. The RMSD reached a stable average within the first 5 ns, and the protein secondary structure indicated stable fluctuations of the relevant domains for preserving the protein fold. Understanding the regulation mechanism is important for developing new inhibitors of the enzyme activity.

Lucio Peña Zarate lucian_marcus@hotmail.com

La seda de araña esta conformada por una serie de proteínas, que se encuentran almacenadas en forma líquida y altamente solubles en agua en las distintas glándulas de la araña. En datos experimentales, se ha estudiado una de estas glándulas, específicamente la Ampulácea mayor que forma la seda estructural, a partir del ensamblaje de espidroina tipo 1 que son secuencias repetitivas de spidroin y un dominio no repetitivo NT-terminal el cual es muy importante para la prevención del auto ensamblaje prematuro de spidroin el cual regula la formación de seda estructural, a través de la modificación del pH e interacciones moleculares. Por lo cual se utilizó la dinámica molecular para simular este dominio NT-terminal, para entender su comportamiento en agua dentro de la Ampulácea mayor y comparar su comportamiento al introducir 1,2-Ethenediol y Di(Hydroxyetil)ether. Y así comprender si estas interacciones, con estos dos compuestos son los responsables del comportamiento del dominio NT-terminal en el auto ensamblaje de spidroin.

Solvation Thermodynamic Properties of Hydrogen Sulfide in [C₄mim][PF₆], [C₄mim][BF₄], and [C₄mim][Cl] Ionic Liquids, determined by Molecular Simulations

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Joel Sánchez-Badillo[†], Marco Gallo^{†*}, Sandra Alvarado[‡], Daniel Glossman-Mitnik[‡]

[†]Facultad de Ciencias Químicas, Universidad Autónoma de San Luis Potosí (UASLP), Av. Manuel Nava No. 6, Zona Universitaria, San Luis Potosí, S.L.P. 78210, México.

[‡]Centro de Investigación en Alimentación y Desarrollo (CIAD), A. C., Av. Cuarta sur No. 3820, Fracc. Vencedores del Desierto, 33089 Unidad Delicias, Chihuahua México.

[‡]Laboratorio Virtual NANOCOSMOS, Departamento de Medio Ambiente y Energía, Centro de Investigación en Materiales Avanzados, Chihuahua, Chih. 31136, México.

Acidic gases such as carbon dioxide (CO₂) and hydrogen sulfide (H₂S) are considered contaminants in the natural gas mixture. Hydrogen sulfide is a toxic and corrosive compound, and their emissions to the atmosphere must be minimized using an absorption process with solvent.

The degree of solubility is the amount of solute retained by the solvent. The solubility can be quantified using the Henry's constant (k_H), free energy of solvation (ΔG_{sol}), or the excess chemical potential (μ^{ex}). For the appropriate selection of a solvent is important also to calculate other thermodynamic properties such as enthalpy (h^{ex}) and entropy (s^{ex}) of solvation (thermodynamic excess properties).

In this work we determine the Henry's constant and the excess thermodynamic properties (h^{ex} and s^{ex}) for the solvation of H₂S in [C₄mim][PF₆], [C₄mim][BF₄], and [C₄mim][Cl] ionic liquids at 298.15 K and 1 bar, using Free Energy Calculations^[1] (FEP) and the Bennet Acceptance Ratio^[2] (BAR) scheme.

The calculated thermodynamic properties are in agreement with existing experimental values^[3,4] except for the H₂S-[C₄mim][Cl] system due to the lack of experimental information at the simulated conditions. The [C₄mim][Cl] ionic liquid displayed the best solvent properties for removing H₂S since it has the highest affinity with the gas specie (lowest free energy of solvation).

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A Comparison of different Force Fields for calculating the [C₄mim] [BF₄] Vapor-Liquid Equilibria using Molecular Simulations.

Sandra G. Hernández¹, Joel Sánchez-Badillo¹, Raúl González-García¹, Pablo López², Marco Gallo^{1*}

¹Facultad de Ciencias Químicas, Universidad Autónoma de San Luis Potosí (UASLP), Av. Manuel Nava No. 6, Zona Universitaria, San Luis Potosí, S.L.P. 78210, México.

²Facultad de Ingeniería en Tecnología de la Madera, Universidad Michoacana de San Nicolás de Hidalgo (UMSNH), Francisco J. Múgica S/N, Colonia Felicitas del Río, Morelia, Michoacán, 58030, México.

In recent years, Ionic liquids (ILs) have received considerable attention due to the variety of applications in technology and scientific areas (catalysis^[1], separation processes^[2], heat transfer fluids^[3], etc.). Their physical and chemical properties depend on the nature of the cation-anion combination. The limitless number of combinations permits designing ILs with different properties and aimed at specific applications.

Molecular Simulations provides an alternative way to explore the IL properties, due to the difficulties associated with carrying experiments at high temperatures and high pressures. Nevertheless the quality of the thermodynamic properties obtained using molecular simulations depends strongly on the quality of the Force Field employed. A first validation to develop high-quality Force Fields is the reproduction of the Vapor-Liquid Equilibrium curve (VLE).

In this work we evaluated different force fields based on OPLS-AA^[4] to calculate the [C₄mim] [BF₄] ionic liquid VLE. The Bonds, angles and dihedrals parameters were obtained with *ab-initio* calculations. The atomic charge were derived using different methodologies: charges derived using ILs dimers^[5], charges derived using an implicit solvent scheme (SMD)^[6], and condensed phase charges derived with the DDEC/c3 method^[7]. These Force Fields were used to calculate the [C₄mim] [BF₄] VLE in a *NVT* ensemble from 300 to 1200 K and compared them with the results obtained from Maginn^[8] and Rane and Errington^[9].

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Dynamics in a Monolayer of Swelling Seeds

Rodrigo Sánchez García
rodrigosg005@gmail.com

Experimental results are presented for the time-evolution of a highly dissipative soft granular submonolayer with non-trivial interactions. The structure exhibits analogies with certain non-equilibrium thermal colloidal systems, yet despite potential applications soft, interacting granular systems have not been as thoroughly reported in the literature as hard ones, and in particular there is a dearth of experimental and simulational work on granular systems with competing attractions and repulsions.

Estudio teórico de los aductos formados entre neurotransmisores y un macrociclo tipo ciclofano.

José Zeferino Ramírez, Ana Gabriela Arvizu, Rosa Elena Navarro

Departamento de Investigación en Polímeros y Materiales, Universidad de Sonora, Blvd. Luís Encinas y Rosales s/n, Colonia Centro, C.P. 83000, Hermosillo, Sonora
jose.ramirez@polimeros.uson.mx

Resumen.

El uso de fármacos cuyo principio activo son moléculas neurotransmisoras es fundamental en el tratamiento de enfermedades como la epilepsia, sin embargo, algunas de éstas moléculas son muy sensibles al medio y se descomponen antes de llegar a la zona del cerebro donde deben ejercer su función. Este problema se ha tratado de resolver mediante el encapsulamiento de los neurotransmisores en macrociclos con cavidades que puedan protegerlos del medio externo.

En este trabajo se presenta la formación de aductos entre un ciclofano derivado de DTPA, denominado BIF11, y los neurotransmisores melatonina, serotonina, L-dopa y dopamina. Las estructuras de los aductos se generaron a partir de una dinámica molecular con el campo de fuerzas AMBER, y posteriormente se reoptimizaron utilizando métodos semiempíricos (PM6, PM6-DH+, PM6-DH2 y PM7).

Stabilizing Interactions in a computer model of a Bax/Bcl-2 heterodimer.

Ana Fernanda Salazar Maldonado anaf.salazarm@gmail.com

Apoptosis is a finely regulated and programmed cellular destruction or death. The main function of this process is to destroy damaged cells and halt diseases such as cancer. Apoptosis is mainly regulated by the Bcl-2 protein family, which consists on at least 25 members. Bcl-2 is a very unique oncogene that does not directly control cellular proliferation. Instead, Bcl-2 blocks cellular death via cytoplasmic contraction, disorganization of the plasmatic membrane, nuclear condensation and endoneucleotic rupture of the DNA processes. Bcl-2 was found to interact with other members of its protein family, forming homodimers and heterodimers that regulate the outer mitochondrial membrane permeability. The first identified homologue of this nature was Bax. In order to understand the interactions between Bax and Bcl-2, we propose a computational model of a Bax/Bcl-2 heterodimer. By studying the nature of the regions that show affinity in this model we may obtain a better understanding of the interactions between members of the Bcl-2 family.

Water Desalination across Nanoporous Graphene Membrane

Francisco Villanueva Mejía,^a José Luis Rivera Rojas,^b Pedro Navarro Santos.^a

^a Instituto de Investigaciones Químico Biológicas, Universidad Michoacana San Nicolás de Hidalgo, Santiago Tapia 403, CP 58000, Morelia, Michoacán, México.

^b Facultad de Ingeniería Química, Universidad Michoacana San Nicolás de Hidalgo, Santiago Tapia 403, CP 58000, Morelia, Michoacán, México.

In this work we analyze the possible development of a new technology for water desalination, we explore the possibilities of a new nano-system that will lead to water desalination with less production cost, addressing the possibility of developing a new nano structured system to obtain a process water desalination, to lower operational cost, this based on conditions of operation of moderate to extreme operating conditions of reverse osmosis. The study consists only of Molecular dynamics simulations, and with these results, we hope to gain a better understanding of what happens at the molecular level in the mass of molecules of water transportation from saline to ion-free water, using capillary forces in a nanostructured system reflecting the processes occurring in a syringe. We propose a system nanostructured similar to a nano-syringe, which uses a membrane of porous Graphene permeable to water molecules, and impermeable to ions and organic pollutants of greater volume to water molecules. The nanostructured system consists of a wall of Graphene, which serve as piston to control the transfer of molecules from one side of the membrane to the other, consisting of a chamber that will contain pure water.

In this work we find that actually by capillary forces in nanostructured systems we can achieve the desalination process. Among the results, find the maximum number of molecules that can be transferred at a determined speed of the plunger, and its noteworthy that efficiencies are greater than those obtained by reverse ósmosis, although it should be noted that these are ideal fluids. Speeds of plunger between 1 and 20 cm/s are able to desalinate the water, higher speeds there is not sufficient adhesion between the plunger and the fluid to be desalinated, there fore the system fails from a high efficiency. Is noted that the flow of water molecules in this process is very high, being several orders of magnitude higher than conventional membranes, mainly due to the high density of pores and the great strength obtained by the capillary system. At the speed of 1 cm/s, we find that the process is reversible, since the accumulated molecules in the Chamber during the process, and the dynamic are the same as those obtained from additional studies of systems in equilibrium.

Authors: Elizabeth Moreno, María Guadalupe Sotelo-Serna, Ramón Castañeda- Priego and Francisco Sastre

Title: Thermodynamic signatures of gelation in adhesive hard-spheres systems

By means of molecular dynamics computer simulations in the microcanonical ensemble with a new method [F. Sastre et al., Phys Rev. E 92, 033303 (2015)], we study the thermodynamic properties of an adhesive hard-spheres system. We particularly find that near to the experimental reported gel transition, the heat capacity seems to exhibit a type of singularity that will allow us to provide, as far as we know, the first thermodynamic signature of gelation in many-body systems with short-range attractive forces.

Flooding tolerance from rice to crops, studies of the structure of the SUB1A-1 protein.

Walter Josué Hernández-Santos¹, Francisco Noe Mendoza-Ambrosio² y Julián Mario Peña-Castro³

¹Ingeniería en Biotecnología, Universidad del Papaloapan, Campus Tuxtepec,

²Laboratorio de Química Teórica, Instituto de Química Aplicada, Universidad del Papaloapan.

³Laboratorio de Biotecnología Vegetal, Instituto de Biotecnología, Universidad del Papaloapan.

SUB1A-1 is transcription factor of the Ethylene Response Factors (ERF's) group VII family. It confers flooding resistance to some rice varieties. Recently this gene was expressed in the model plant *Arabidopsis thaliana* for genetic studies which has shown than this gene has also others biological properties such as oxygen sensor, transcription factor and interaction with other proteins. However, the tridimensional structure has not been determinate due to the difficulty involved in the *in vivo* protein purification and the crystallization required by methods like X Ray diffraction or Nuclear Magnetic Resonance (NMR). In this work we made a numerical analysis to predict the most probable tridimensional structure of SUB1A-1 protein from rice (*Oriza sativa*) using as starting point the model outed by I-Tasser server and adding structural refinement by Molecular Dynamics with the simulated annealing method using GROMACS software. Ssimultaneously we are performing experiments with genetic constructions of this protein expressed constitutively in *Arabidopsis thaliana* to show the importance the biological role of motifs identified in the sequence.

Direct Coexistence Methods to Determine the Solubility of Salts

Authors: Héctor Manuel Manzanilla Granados

Raúl Fuentes Azcatl

Humberto Saint-Martín

José Alejandro

The solubility of NaCl, an equilibrium between a saturated solution of ions and a solid with a crystalline structure, was obtained from molecular dynamics simulations using the SPC/E and TIP4P-Ew water models. Four initial setups on supersaturated systems were tested on sodium chloride (NaCl) solutions to determine the equilibrium conditions and computational performance: (1) an ionic solution confined between two crystal plates of periodic NaCl, (2) a solution with all the ions initially distributed randomly, (3) a nanocrystal immersed in pure water, and (4) a nanocrystal immersed in an ionic solution. In some cases, the equilibration of the system can take several microseconds. The results from this work showed that the solubility of NaCl was the same, within simulation error, for the four setups, and in agreement with previously reported values from simulations with the setup (1). The system of a nanocrystal immersed in supersaturated solution was found to equilibrate faster than others. In agreement with laser-Doppler droplet measurements, at equilibrium with the solution the crystals in all the setups had a slight positive charge.

Re-parameterizing a force field for Formamide molecule

Alexander Pérez de la Luz, José Alejandro.

Departamento de Química, Universidad Autónoma Metropolitana, Iztapalapa, D.F. México.

In molecular simulations the force fields which contain the interaction parameters are essential for a good description of real systems. In this work a methodology of re-parameterization of OPLS/AA (Optimized Potentials for Liquid Simulations all Atoms) force field for Formamide molecule is present. This process was necessary in order to improve results in some specific properties (dielectric constant (ϵ), surface tension (σ) and density (ρ)) and compare with various force fields, e.g. OPLS/AA, GAFF, CHARMM, and GROMOS. This method is systematic and simple, it consists in relating properties with specific parameters of the intermolecular interaction. 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 preliminar study of solubility.

A study of the fully asymmetric spherical electric double layer: a comparison between the semi-punctual and hard-sphere ions models.

Evelyn Angélica Barrios-Contreras¹, Enrique González-Tovar¹, Guillermo Iván Guerrero-García¹

¹Instituto de Física, Universidad Autónoma de San Luis Potosí; México

eangelica.barrios@gmail.com

The arrangement of ions around a charged colloid or surface, immersed in an electrolyte, is called the electric double layer (EDL). Throughout the years, the study of the EDL has rested on diverse models, such as those considering point-ions or the more recent representations that include finite size effects. In particular, an effect of great importance in the analysis of the EDL is, certainly, the asymmetry in size and/or charge of the ionic species. Therefrom, in this work, a theoretical investigation of a colloidal system (in spherical geometry) is performed via two formalisms derived from the Ornstein-Zernike equation. The first one, known as the URMGC theory (Unequal Radius Modified Gouy-Chapman), considers a model of quasi-punctual ions, bearing a distance of closest approach, which introduces “size” contributions in a simple form. The second one, called the HNC/MSA theory (Hypernetted-Chain/Mean Spherical Approximation) is based on a more complete model in which the ions are charged hard-spheres. In the present contribution, we compare and analyze several results of those approaches, e.g., their radial distribution functions, as well as their electrostatic potential and integral charge profiles, for systems with ionic size- and charge-asymmetry. Notable qualitative and quantitative differences between the EDL descriptions associated to the semi-punctual and hard-sphere models are observed.

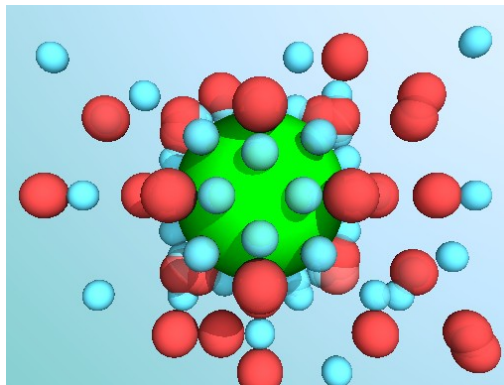


Figure: The spherical electrical double layer.

Structure and Thermodynamics of $\text{CaF}_2(\text{H}_2\text{O})_n$ ($n < 15$) clusters by ab initio method.

Víctor M. Rosas-García, Isabel Sáenz-Tavera, Alcíone García González
Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL.
CP 66451 México E-mail:victor.rosasgr@uanl.edu.mx

We study microhydrated calcium fluoride and its ions at the restricted Hartree–Fock RHF/6-31G* level of theory. A semiempirical molecular dynamics search of progressively more hydrated species provides lowest-energy configurations that are then fully optimized and characterized as energy minima at the RHF/6-31G* level of theory. We discuss the first solvation shells of both calcium fluoride and fluoride anion. QTAIM calculations show critical points for hydrogen bonding. We discuss the total standard enthalpies of hydration for fluoride ion and calcium fluoride at infinite dilution, and whether the dissociation of hydrated calcium thiosulfate at infinite dilution is an endothermic or exothermic process.

Adsorción de Arsénico en la superficie de Pirita (100)

José Miguel Mora Fonz¹, C. Richard A. Catlow²

¹Universidad Juárez Autónoma de Tabasco, División Académica de Ciencias Básicas, Car. Cunduacán-Jalpa km 1 Cunduacán Tabasco CP 86690

²Department of Chemistry, University College London, 20 Gordon St., London WC1H 0AJ, UK
*jmiguel.mora@ujat.mx

La interacción de diferentes especies de arsénico con la superficie ideal de (100) de pirita se modelan usando la Teoría de Funcionales de la Densidad, para tener una mejor comprensión de la movilidad de arsénico de minerales de pirita, que contienen este elemento. La pirita ocurre en depósitos naturales que pueden contener diferentes niveles de arsénico.^[1] Se ha propuesto que el arsénico sustituye el sulfuro de la pirita^[2] y cuando este mineral es expuesto a condiciones oxidantes, el mineral se disuelve exponiendo el elemento venenoso. Mediante este proceso el arsénico puede contaminar depósitos de agua, lo cual puede ser un riesgo potencial para personas o animales de ser utilizado.^[3] El mecanismo por el cual el arsénico se incorpora y se remueve de la pirita no se conoce completamente. En este estudio, para resolver el problema, se emplea el funcional de DFT rPBE con conjuntos base de pseudopotenciales de ondas planas implementados en el código CASTEP, que se emplea con éxito en este sistema.^[2, 4] La adsorción de moléculas de agua y oxígeno se calculan y comparan con estudios previos, y la adsorción de especies de arsénico presentes en solución se investiga para conocer sus implicaciones en la remoción de este elemento.

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EVALUACION DE LA CAPACIDAD ANTIOXIDANTE MEDIANTE CUPRAC ELECTROQUIMICO EN EXTRACTOS DE ZANAHORIA NEGRA Y GARAMBULLO: EFECTO DEL TETRAETILORTOSILICATO (TEOS) Y CONTENIDO DE AZUCARES REDUCTORES.

María de los Angeles Díaz Victoria

Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Parque Tecnológico Querétaro Sanfandila, 76703 Sanfandila, Pedro Escobedo, Querétaro.

Extractos de garambullo y zanahoria negra fueron analizados mediante la técnica CUPRAC (Cupric Reducing Antioxidant Capacity) electroquímico para evaluar su capacidad antioxidante total en ausencia y presencia de un compuesto de Silicio llamado TEOS (tetraetilortosilicato), que actúa como estabilizante o retardante en la degradación de pigmentos. Estos extractos contienen agentes antioxidantes como son antocianinas y betalainas. Se encontró una disminución de la CAT (capacidad antioxidante total) para las muestras frescas que contienen TEOS al ser comparadas con los extractos que no lo contienen, se realizó nuevamente la prueba pasada una semana a las mismas muestras, bajo las mismas condiciones de operación donde se puede observar que la degradación de los antioxidantes AO fue menor en presencia de TEOS. Se analizaron nuevas muestras en ausencia de azúcares reductores, mostrando una disminución importante en la señal de corriente de pico, lo que indica que la técnica CUPRAC es capaz de detectar y cuantificar azúcares reductores en muestras de jugos.

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Precise Delivery in Nanomechanical Systems Using Graphene/Graphite Monoliths

Jose Luis Rivera, and Roberto Guerra-Gonzalez

Facultad de Ingeniería Química, Universidad Michoacana de San Nicolás de Hidalgo, 58000 Morelia,
MICH, México

The precise delivery of graphene sheets through a ordered set of graphite monoliths forming a lane for the transport of the graphene sheets was investigated using Molecular Dynamics simulations. The graphite monoliths consisted of 20 graphene sheets having a surface of 2 x 2 nm, and one of those sheets was rigid and its position was fixed, making the average position of the monolith also fixed. The monoliths in the lane were located at separations of 6.8 Å between the centers of the atoms that form the edge of the graphene sheets forming the graphite monoliths. One graphene sheet of dimension 1 x 1 nm moved through the lane of graphite monoliths using an initial momentum, such momentum was created by pulling the moving graphene at a position where there is a small overlap between the moving graphene sheet, and the first graphite monolith forming the lane of monoliths. The strength of the initial moment was tuned through the control of the initial overlapping between the moving graphene sheet and the first graphite monolith. As the moving graphene sheet is transported through the monoliths lane, the average velocity of the moving graphene sheets until the movement stops. We study the displacements of the graphene sheets and report profiles of the moving graphene positions, velocities, acceleration, and interactions forces with the graphite monoliths.

TRANSPORT PROPERTIES OF POLAR SOLVENTS

Edith Nadir de Jesús González, Jorge López Lemus.

Facultad de Ciencias. Universidad Autónoma del Estado de México.

Liquid densities for polar solvents such as acetone and ethanol were estimated by means of molecular dynamics simulations. These molecular simulations were performed in an isothermic-isobaric ensemble. Molecular interactions were described by OPLS-AA force field. This force field cannot reproduce the experimental dielectric constant. Furthermore, transport properties such as shear viscosity and self-diffusion were estimated using the force field above mentioned. Then, charges for each atom were calculated again with the intention of reproducing the experimental dielectric constant. Finally, a comparison among transport properties estimated with both force fields was carried out.

Shifting the coexistence temperature to higher temperatures with an external electric field observed in methane hydrate

D. P. Luis ^a, J. López-Lemus ^b, H. Saint-Martin ^c

^a Centro de Ingeniería y Desarrollo Industrial, Av. Playa Pie de la Cuesta No. 702. Desarrollo San Pablo, Querétaro, Querétaro, 76125, México

^b Facultad de ciencias, Universidad Autónoma del Estado de México, Toluca, CP 50295, México.

^c Instituto de Ciencias Físicas, Universidad Autónoma de México, Av. Universidad s/n, col. Chamilpa, Cuernavaca, Morelos , 62210, México

In the present work we used molecular dynamic simulations in the equilibrium NPT ensemble to examine the effect of an external electric field on the three-phase coexistence temperature of methane gas, liquid water and methane hydrate. For these simulations, we used the TIP4P/Ice rigid water model and a single-site model for methane. The simulations were implemented at a pressure of 400, over temperatures ranging from 285 K to 320 K. The application of an external electric field in the range of 0.1V nm^{-1} to 0.9V nm^{-1} caused the effect of the thermal vibrations of the water molecules to become attenuated. This resulted in a shift of the three-phase coexistence temperature to higher temperatures. Electric fields below this range did not cause a difference in the coexistence temperature, and electric fields above this range enhanced the thermal effect. The shift had a magnitude of around 20 K.

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Solubility of paracetamol in water

Hugo Flores Ruiz¹, Arlette Mendez², Edgar Nuñez¹ and José Alejandro¹

¹Universidad Autónoma Metropolitana - Iztapalapa

²Catedra Conacyt-Universidad Autónoma de San Luis Potosi

The solubility of paracetamol in water at room temperature is studied by means of molecular dynamics simulations. In order to set up paracetamol, we use principle of transferability since we assemble paracetamol from phenol and acetamide molecules. We have found out that the solubility of paracetamol in water can be increased by adding formamide and acetamide. For water we are using the TIP4P/ε model. In the case of paracetamol, we are using OPLS parameters for acetamide and Trappe parameters for phenol.

CONSTRUCCIÓN Y EVALUACIÓN DE FUNCIONAMIENTO DE UN SISTEMA MÓVIL ELECTROQUÍMICO PARA TRATAMIENTO DE CONTAMINANTES EN AGUAS SUPERFICIALES.

BEATRIZ GARCIA iq.beatrizgarcia@hotmail.com

Las aguas de los cuerpos superficiales y subterráneos se contaminan por las descargas sin tratamiento previo de aguas municipales e industriales, así como por los arrastres que provienen de las zonas que practican actividades agrícolas y pecuarias.

El agua es uno de los recursos más importantes para la vida en el planeta, el ser humano depende de su disponibilidad no solamente para consumo doméstico, si no para el desarrollo de todas sus actividades.

En México durante los últimos años el problema de la disponibilidad de agua ha crecido exponencialmente, debido al incremento en la contaminación del recurso, la red de abastecimiento y sus deficientes condiciones. La mayoría de los contaminantes presentes en aguas residuales son persistentes, es decir, no son fácilmente tratables por métodos convencionales, por lo que el desarrollo de nueva tecnología que permita dar solución a este problema es una necesidad actual de la sociedad.

Grupos de investigación alrededor del mundo desarrollan día con día nuevos procesos y técnicas que permitan la disminución o en mayor medida la eliminación de los contaminantes en las aguas con la finalidad de ser re-utilizadas.

En los últimos diez años, los procesos electroquímicos han demostrado su eficiencia para la degradación de compuestos orgánicos en aguas residuales.

El presente proyecto plantea la construcción de un dispositivo móvil con acoplamiento de dos tecnologías, una electroquímica y tecnología foto-voltaica. Se pretende la generación ``in situ`` del peróxido de hidrogeno electroquímicamente, a partir de la reacción de reducción de oxígeno en el medio, empleando como cátodo fieltro de carbón. El cual fue desarrollado en el CIDETEQ.

Se empleó un contaminante prueba, colorante naranja II para el desarrollo de los experimentos.

Los resultados obtenidos muestran que se obtiene decoloración al terminar el experimento.

Simulation of a BCL-XL complex. Eduardo Piña Gómez del Campo, Francisco Javier García Pérez, Lizbeth Aldonza De la Torre López, Eduardo Piña Gómez del Campo, Rosaura Palma Orozco, Jorge Luis Rosas Trigueros. Laboratorio Transdisciplinario de Investigación en Sistemas Evolutivos, SEPI de la ESCOM del Instituto Politécnico Nacional. jlrosas@ipn.mx

Abstract

B-cell lymphoma-extra-large (Bcl-xl) is a member of the Bcl-2 family of proteins, and acts as a pro-survival protein by preventing the release of mitochondrial contents such as cytochrome c.

Similar to Bcl-2, it has been implicated in the survival of cancer cells. Bcl-xL is known to be over-expressed in hematopoietic disorders such as polycythemia vera. It is also a major survival factor responsible for an estimated half of the total survival "signal" proerythroblasts must receive in order to survive and become red cells. The BH3 domain is common to all Bcl-2 family members and has been shown to play a role in the interaction between these proteins. In this work, a complex Bcl-xl/BH3 is submitted to molecular dynamics simulations with the aim to better understand the interactions involved.

Computer simulation of two BAX monomers at high pH, Lizbeth Aldonza De la Torre López, Francisco Javier García Pérez, Eduardo Piña Gómez del Campo, Rosaura Palma Orozco, Jorge Luis Rosas Trigueros. Laboratorio Transdisciplinario de Investigación en Sistemas Evolutivos, SEPI de la ESCOM del Instituto Politécnico Nacional. jlrosas@ipn.mx

BAX is a Bcl-2 family proapoptotic protein. BAX has the ability to become a killer protein in response to cellular stress. This transformation requires conformational changes that allow BAX to form homodimers and heterodimers with other members of the Bcl-2 family. These complexes have been found to regulate the liberation of apoptogenic factors located inside the mitochondria. The activation of BAX can be triggered in several ways, including high pH. However, previous work suggests that high pH might not be enough to activate a single BAX monomer. In this work, we present a simulation of two BAX monomers at high pH. The behavior of this model may help understand the interactions involved in early stages of BAX activation.

Extended simulation of a BAX/BH3 complex. Francisco Javier García Pérez, Lizbeth Aldonza De la Torre López, Eduardo Piña Gómez del Campo, Rosaura Palma Orozco, Jorge Luis Rosas Trigueros. Laboratorio Transdisciplinario de Investigación en Sistemas Evolutivos, SEPI de la ESCOM del Instituto Politécnico Nacional. jlrosas@ipn.mx

Bax is a proapoptotic member of the Bcl-2 family, due to its ability to become a killer protein. The interaction between Bax and BH3 can trigger the activation of the proapoptotic function of Bax. In this work, an atomistic model of a BAX/BH3 complex is simulated to investigate its behavior, focusing on the effects of this interaction on the structure of BAX. Previous work produced a model of Bax with BH3, where BH3 started at a position and approached the hydrophobic groove of Bax in a short molecular dynamics simulation, but no dramatic conformational changes were observed. In this work, the simulation is extended with the aim to improve the understanding of the interaction between these proteins.

Non-conformal effects on interfacial and critical properties of simple fluids.

Manuel Fuentes Herrera.

Universidad Autónoma del Estado de México.

Molecular simulations in the canonical and isothermal -isobaric ensembles were developed to study the effect of the shape - non-coformality - of intermolecular potential about critical and interfacial properties of model fluids. The molecular interaction was modeled through of a family of potentials proposed by a theory called ANC (Approximate Non-Conformal Theory) which depends of the usual scale parameters of size and energy. This theory also introduce a new form parameter called softness that module the shape of molecular potential in their repulsive and attractive parts simultaneously. A extended version of ANC-potentials were used in this research, where the softness is considered independent in the repulsive and attractive parts of the interaction. This flexibility of the theory allows to explore the role of the molecular interactions on critical and interfacial properties separately.

CHEMICAL REACTIVITY OF ALKANOLAMINES

J.G. Bringas-González¹, J. López-Lemus¹, R. López-Rendón¹, R. Vargas-Fosada²

¹*Facultad de Ciencias, Universidad Autónoma del Estado México, México.
Instituto Literario No. 100. C.P. 50000, Toluca, Estado de México*

²*Departamento de Química, Universidad Autónoma Metropolitana de Iztapalapa.
San Rafael Atlixco No. 186, Col. Vicentina, Iztapalapa, 09340, México.*

We calculated the chemical reactivity of the alkanolamines: Monoethanolamine (MEA), 2-Methylaminoethanol (MAE), Dimethylaminoethanolamine (DMMEA) and 2-amino-2-methyl-1-propanol (AMP) by Density Functional theory (DFT). The electronic affinity, ionization energy, condensed Fukui functions and the electron donors and acceptors power (local and global) were estimated. These calculations were performed by using the B3LYP and PBE0 functionals with the 6-31+g(d,p), 6-311++g(2d,2p) and aug-cc-pVTZ base set. Based on the obtained results, the reactivity of the alkanolamines studied here were discussed. All this information can be useful for the enhancement of the sweetening process of natural gas.

COMPUTATIONAL STUDY OF ISONICOTINAMIDE-FORMAMIDE COCRYSTAL

Frank José Salas¹, Edgar Núñez-Rojas¹, José Alejandro¹

¹Departamento de Química, División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco 186, Col. Vicentina, C.P. 09340 México, D.F.

Abstract

Cocrystal formation is a useful strategy in order to improve both solubility and bioavailability of poorly soluble drugs. A principal aspect in this formation is the hydrogen bond, which is responsible for the majority of directed intermolecular interactions in molecular solids. Cocrystallization is a manifestation of directed self-assembly of different components and it has been described for several organic substances over the years.

The isonicotinamide-formamide cocrystal structure was preserved by using Molecular Dynamics. In this case it was used a set of interaction parameters for the force field which were obtained from previous works of both, the formamide and the pyridine molecules. In simulations the crystalline properties were important since the structure was sensible to the shape of the simulation cell (the triclinic one). Distances and angles were determined and results were in agreement with experimental results. It is important to mention that cocrystal formation was not possible to reach by Annealing methodology from a molecular system in which molecules were placed randomly. The reason for this could be that changes in temperature were not adequately chosen. However, the structure preservation is also a way to validate a force field.

Conformational analysis of insulin in the microseconds timescale

Óscar Olvera Neria¹, Ana Carmen Estrada Real¹, Ivonne Reyes Molina¹, Julio César González Torres¹, Roberto López Rendón², Óscar N. Ventura Pérez³, Patricia Saenz Mendez³, Aline Katz Wisel³

¹ Área de Física Atómica Molecular Aplicada (FAMA), CBI, Universidad Autónoma Metropolitana-Azcapotzalco, Av. San Pablo 180, Col. Reynosa Tamaulipas, Mexico, D.F. 02200, Mexico.

² Laboratorio de Bioingeniería Molecular a Multiescala, Facultad de Ciencias, Universidad Autónoma del Estado de México, Av. Instituto Literario 100, Toluca, Mexico.

³ Facultad de Química, UdelaR, Avda. Gral Flores 2124, CC1157, 11800 Montevideo, Uruguay.

Type 2 diabetes mellitus is the leading cause of death in Mexico; in addition to the standardized mortality rate it has increased steadily from 1990 to the present day and consumed 20% of the health sector budget, so configured diabetes mellitus as a public health problem. Efforts to understand the disease from all possible aspects: clinical pharmacology, public health, molecular biology, ultimately contribute for improving the quality of life of people with the disease and develop strategies for early detection of diabetes and the subsequent application of preventive therapies. The first step to study the insulin resistance is to characterize the structure of the 51 amino acids that conform the human insulin. We perform molecular dynamic calculations in the microseconds timescale using the program ACEMD. These calculations generated about one billion of configurations, which were analyzed with Markov state models (MSMs) implemented in the program MSMBuilder to map the insulin conformational space and for determining the matrix of transition probabilities to identify the most stable conformations of insulin.

Parametrisation of a force field of acetamide for simulations of the liquid phase

Jorge A. Aguilar-Pineda, G. Arlette Méndez-Maldonado, Edgar Núñez-Rojas and José Alejandro

Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, México Distrito Federal, México

Abstract

Molecular dynamics simulations are performed to develop new parameters for acetamide using a systematic procedure proposed by Salas *et al.*, where the atomic charges were fitted to reproduce the experimental dielectric constant and the Lennard-Jones parameters to match the surface tension and density. The parameters for formamide recently calculated by Pérez *et al.* were used to obtain the new parameters of acetamide where atoms of the amine group and carbon kept the same intermolecular parameter values in both molecules. The parameters of the methyl group, taken as united atom, and the oxygen atom were fitted to reproduce the dielectric constant, surface tension and density at 358.15 K. The new set of parameters, based on the optimised potential for liquids simulations with all atoms, was able to predict results of the target properties as a function of temperature as a pure component and the dielectric constant and density of binary mixtures with water and formamide as a function of acetamide concentration at 298.15 K. The polymer chains formed by hydrogen bond interactions were analysed to understand the maximum of dielectric constant in acetamide-water mixtures.