

Desarrollo y Aplicaciones de AMOEBA-IL

G. Andrés Cisneros

Department of Chemistry, University of North Texas, Denton, TX, 76206

Presentaremos el desarrollo de parámetros para AMOEBA para líquidos iónicos (LI) usando multipolos distribuidos derivados del Gaussian Electrostatic Model (GEM). Aplicaciones de este nuevo potencial multipolar/polarizable para investigar propiedades de diferentes mezclas de LIs basadas en cationes de imidazolio y de pirrolidinio, así como una reacción de protección de anilina serán discutidas.

Pharma-Dock, another docking server based on free software

César Millán Pacheco

Facultad de Farmacia, Universidad Autonoma del Estado de Morelos

Molecular docking algorithms have been used as a tool to test a hypothesis about the binding affinity of small ligands to pharmaceutical targets. Unfortunately, user accessibility to this kind of software made them very popular among users that require a fast explanation for some experiments. There exist any kind of online tutorials to learn how to use docking software without any recommendation about statistical considerations or cautions that as user must have to use them.

Here, we present a web server that will try to correct this issue. Pharma-dock is a web server based on free software that makes use of molecular dynamics simulations to improve the statistical results. Users may choose to use crystallographic coordinates, minimized structures, last structure or center-cluster structure based on clustering analysis from the molecular simulation as receptor structure and if they will like to use the entire protein (blind docking) or binding site coordinates (directed docking). Also, to estimate the statistical error associated with individual docking runs any docking submitted may report at least 3 (3, 10, 100 and 1000) independent docking experiments. Documentation associated with Pharma-dock gives a detailed explanation about the advantage to use these parameters.

TITLE: The role played by interactions in the assembly of active colloids

ABSTRACT:

Active matter systems are composed of constituents that consume energy in order to move or exert mechanical forces, constantly driving themselves away from equilibrium [1]. Examples of active particles are living, such as bacteria, or artificial, such as active colloids [2,3].

Experiments on spherical man-made self-propelled colloids have shown that active particles present interesting emergent collective properties [4–6], such as motility-induced phase separation (MIPS), involving spontaneous assembly of particles due to the persistence of their direction of motion [7]. An example of colloids undergoing MIPS under suitable conditions are Active Brownian Particles (ABP), i.e. self-propelled Brownian particles interacting with each other via a purely repulsive potential [8].

In order to design novel functional materials, one might need to gain control on the self-assembly process of active colloids.

With this goal in mind, we have explored the competition between activity and a broad range of interactions between active colloids, ranging from isotropic (strongly repulsive [9,15,17], attractive [10,11], micelle-inducing [12]) to anisotropic (Janus-like [13]), unravelling the relevance of hydrodynamics [11,14,16].

REFERENCES

- [1] C. Bechinger et al. *Rev. Mod. Phys.* 88, 045006 (2016).
- [2] W.F. Paxton et al. *Chem. Commun.* 441, 3 (2005).
- [3] S. Fournier-Bidoz et al. *J. Am. Chem. Soc.* 126, 13424 (2004).
- [4] S. Thutupalli, R. Seemann, S. Herminghaus *New J. Phys.* 13, 073021 (2011).
- [5] D. Nishiguchi, Masaki S. *Phys. Rev. E* 92, 052309 (2015).
- [6] I. Buttinoni, J. Bialké, F. Kümmel, H. Löwen, C. Bechinger, T. Speck. *Phys.Rev. Lett.* 110, 238301 (2013).
- [7] M.E. Cates, J. Tailleur. *Annu. Rev. of Condens. M3tt. Phys.* 6, pp. 219–244 (2015).
- [8] S.Mallory, C.Valeriani and A.Cacciuto *Annual review of Physical Chemistry*, 69 59 (2018)
- [9] Diego Rogel Rodriguez, Francisco Alarcon, Raul Martinez, Jorge Ramirez, and Chantal Valeriani, in preparation (2018)
- [10] B. Mognetti, A. Saric, S. Angioletti-Uberti, A. Cacciuto, C. Valeriani and D. Frenkel *Phys.Rev.Lett.*, 111 245702 (2013)

- [11] F.Alarcon, C.Valeriani and I.Pagonabarraga Soft Matter 10.1039/C6SM01752E (2017)
- [12] C.Tung, J.Harder, C.Valeriani and A.Cacciuto, Soft Matter 12 555 (2016)
- [13] S.Mallory, F.Alarcon, A.Cacciuto and C.Valeriani New Journal of Physics (2017)
- [14] F.Alarcon, E.Navarro, C.Valeriani and I.Pagonabarraga, PRE in press (2019)
- [15] J.Harder, S.Mallory, C.Tung, C.Valeriani and A.Cacciuto, J.Chem.Phys. 141 194901 (2014)
- [16] R.Martinez, F.Alarcon, D.R.Rodriguez, J.L.Aragones and C.Valeriani, EPJE 41 91 (2018)
- [17] Diego Rogel Rodriguez, Francisco Alarcon, Raul Martinez, Jorge Ramirez, and Chantal Valeriani, in preparation (2019)

CO-AUTHORS

Francisco Alarcon	Universidad Complutense de Madrid
Eloy Navarro	University of Barcelona
Ignacio Pagonabarraga	University of Barcelona/CECAM
Stewart Mallory	Caltech
Angelo Cacciuto	Columbia University

**An undiscovered code in the intrinsically disordered proteins:
Phosphorylation as control of ligand binding and protein structure.**

Eduardo Villarreal-Ramirez.

Tissue Bioengineering Laboratory, DEPeI, Faculty of Dentistry, National Autonomous University of
Mexico, Mexico Distrito Federal, Mexico.

Intrinsically Disordered Proteins (IDPs) or Intrinsically Disordered Regions (IDRs) have gained ever-increasing relevance during the last years due to their atypical properties. IDPs/IDRs are lacking a tridimensional structure on physiological conditions, and they are able to adopt highly dynamic conformations, allowing in most cases binding to several partners. IDPs play diverse and essential roles in biological systems as signaling processes, transcription, including mineralization of bone and teeth. In globular proteins, phosphorylation can promote conformational changes and also can alter surface recognition. This knowledge has been understood in depth by crystallographic studies. However, IDPs can not form protein crystals. Many IDPs are highly phosphorylated via post-translational modifications. Phosphorylation in IDPs induce conformational changes, promote order-disorder transitions, and modulate binding via electrostatic interactions with partners. Nevertheless, the evidence in the literature regarding the role of phosphorylation on the conformational kinetics of IDPs is not conclusive, and which is the effect on molecular recognition with their partners is still elusive. Previous studies have shown that phosphorylation on IDPs has a profound effect on the flexibility that is essential for performing their functions and allowing them to explore different conformations. By performing molecular dynamics simulations (MD) of several IDPs, showed the phosphorylated version of them showed higher affinity to their partners and a more organized structure. The change to a more-ordered structure after phosphorylation and interactions with their partners was verified by circular dichroism, small-angle scattering, and vibrational spectroscopy.

Weak interactions in DNA: a DFT study in CpG-island-like chains

Jorge Gutiérrez-Flores, Enrique Hernández-Lemus, Fernando Cortés-Guzmán, Estrella Ramos

Abstract

Weak interactions play a fundamental role in the stability and structure of a large number of molecules. Such is the case of the hydrogen bond and π - π stacking interactions in the deoxyribonucleic acid (DNA). This work study the effect of the number of base pairs (chain length) on both hydrogen bonds and π - π stacking, using as model GC-rich chains based on the CpG islands sequence (CpG island-like chains). We found that there is no relevant effect due to the presence of other base pairs since no significant changes in hydrogen bond and π - π stacking energies were predicted. However, anticooperative effects were observed for both hydrogen bonds and π - π stacking interactions. These results are in contrast with those of TATA-box-like chains since cooperative and additive effects were found for both hydrogen bonds and π - π stacking, respectively. Finally, based on the chemical hardness and density of states, we are able to conclude that proteins may interact easier with GC-rich chains because 8GC is less hard than 8TA and, besides, its last unoccupied levels are energetically outer than those from 8TA, delving deeper into the biological differences between the TATA box and CpG island promoter regions and shedding light on the relevance, from a biological viewpoint, of noncovalent interactions, electronic and chemical properties of the different kinds of DNA sequences. We also notice that all of our work was performed under the DFT framework included in DMol3 code (M06-L/DNP).

Biofilms under hydrodynamic stress.

Francisco Alarcón^{1,2}, Valentino Bianco³, Pin Nie⁴, Luis Dinis², Massimo P. Ciamarra⁴, María A. Canales³,
Ivan Lopez-Montero³, Belén Orgaz⁵ and Chantal Valeriani²

¹*Departamento de Ingeniería Física, División de Ciencias e Ingenierías,
Universidad de Guanajuato, Loma del Bosque 103, 37150 León, Mexico*

²*Departamento de Estructura de la Materia, Física Térmica y Electrónica,
Facultad de Ciencias Físicas, Grupo Interdisciplinar de Sistemas Complejos,
Universidad Complutense de Madrid, 28040 Madrid, Spain*

³*Departamento de Química Física, Facultad de Ciencias Químicas,
Universidad Complutense de Madrid, 28040 Madrid, Spain*

⁴*School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore*

⁵*Sección Departamental de Farmacia, Farmacia Galénica y Tecnología Alimentaria,
Facultad de Veterinaria, Universidad Complutense de Madrid, 28040 Madrid, Spain*

Biofilms are communities of microorganisms which excrete an extracellular polymeric matrix. We present experimental data of biofilm population growth [1] at different times in different growing conditions. In particular, stirring of culture medium greatly enhances biofilm growth. Bacterial population dynamics can be satisfactorily modelled by a simple population dynamics model with reasonable assumptions. Using the model we can approximately explain the different growth behavior observed in shaking versus static conditions. We have additionally developed numerical simulations to study biofilm development where bacteria interact via an effective depletion force produced by excreted polymers.

Once the bacteria attach to the surface or interface they produce a gluey extracellular polymeric network (termed EPS) composed basically by polysaccharides and proteins. Bacteria then are embedded in this extracellular network or matrix (ECM). As an analogy to a typical problem in soft matter physics: the rigid bacteria can be seen as active colloids, whereas the extracellular matrix as a cross-linked polymer gel [2]. This approach is useful for understanding the structure, mechanics, and dynamics of the biofilm. Since, the mechanics of well-defined soft materials can provide insight into the mechanics of biofilms and, in particular, the viscoelasticity.

References:

- [1]. R. J. Allen and B. Waclaw, Reports on Progress in Physics 82, 016601 (2019).
- [2]. J. N. Wilking, T. E. Angelini, A. Seminara, M. P. Brenner and D.A. Weitz, MRS Bulletin 36(5), 385-391 (2011).

COMPUTATIONAL STUDY OF PHARMACEUTICAL COCRYSTAL

Frank José Salas Sánchez,¹ Edgar Núñez¹ and José Alejandro

¹ Departamento 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.

Keywords: cocrystal, dielectric constant, parameterized, stability, hydrogen bonds

INTRODUCTION

The Biopharmaceutics Classification System (BCS) is a system to differentiate the drugs on the basis of their solubility and permeability, in order to establish its potential absorption properties after their administration by extravascular, primarily orally. This classification takes into account the dose of drug to be administered to achieve therapeutic effects as it relates to the dissolution in aqueous media, which to be acceptable must not exceed the saturation concentration. This is because the drug must be dissolved to be absorbed state. However, there are drugs that have low solubility, low permeability and high hygroscopicity. Consequently significantly decreases the bioavailability of the drug. The solubility is one of the parameters that determine the bioavailability of a drug. Hence in the pharmaceutical industry provides the ability to alter their physicochemical properties without compromising the structural integrity of IFA, the latter responsible for the therapeutic effect on the body.

In this paper a methodology is shown in order to understand the stability and try to predict the formation of a cocrystal. We will use own programs and Gromacs MD simulations to develop as a starting point and potential parameters OPLS / AA (Optimized Potentials for Liquid Simulations). The formation of cocrystals is due to the formation of hydrogen bonds, so it is convenient to analyze whether OPLS / AA parameters correctly describe electrostatic interactions. The macroscopic fluid property that is related to these interactions is the dielectric constant was verified that this potential does not reproduce this property. Therefore loads, geometry and parameters of Lennard-Jones (LJ) was modified to reproduce the properties of the liquid-vapor equilibrium and surface tension. This study was conducted for the cocrystal formic acid/pyridine, isonicotinamide/formamide and nifedipine/dimethylsulfoxide. To observe the formation of the crystal, the radial distribution function was used to measure the distances of the atoms that form hydrogen bonds and angles formed by the molecular species. On the other hand, it is possible to stabilize cocrystal with force field parameters developed to simulate liquids. The dielectric constant of the components, wich is important to simulate polar systems, does not play a key role in the simulation cocrystal although the hydrogen bonding interactions are the driving force to form these systems. The advantage of the new force fields parameters that reproduce the dielectric constant will be seen in simulations of cocrystal in contact with polar solvents in liquids, that is the case of several drugs which are prepared as cocrystals and then mixed with a solvent such as water.

Cocristales moleculares – Definición y breve panorama de aplicaciones

Herbert Höpfl

Centro de Investigaciones Químicas, Instituto de Investigación en Ciencias Básicas y Aplicadas
Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Cuernavaca 62209, Morelos.

E-mail: hhopf@uaem.mx

Es objetivo de la *Ingeniería de Cristales* entender los factores que gobiernan la organización de compuestos moleculares en el estado cristalino por medio de la formación de enlaces no-covalentes (supramoleculares), y de allí inferir en la predicción y alteración de la estructura cristalina. Las propiedades físicas y fisicoquímicas de un sólido, tales como punto de fusión, densidad, color, conductividad térmica y eléctrica, magnetismo, solubilidad, etc., dependen de la estructura que adoptan las moléculas que lo constituyen y se pueden modificar al cambiarla (Figura 1). Esto es relevante para la Ciencia de Materiales, las Ciencias Farmacéuticas, entre otros. Una de las opciones más recientes para abordar esta temática consiste en la generación de *cocristales*. La conferencia explicará con más detalle que son cocristales y mostrará algunos ejemplos que evidencian el impacto que pueden tener en diferentes áreas de la Ciencia.

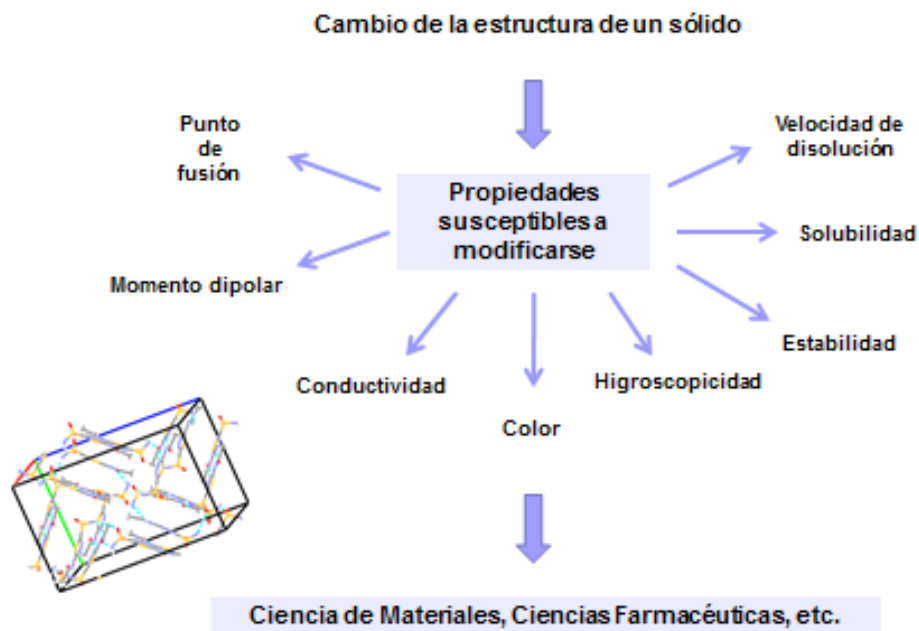


Figura 1. Algunas propiedades que pueden modificarse mediante el cambio de la estructura de un sólido cristalino.

Nanodomain formation in the lipidic bilayer, origin, modulation and biological relevance.

Iván Ortega Blake
Instituto de Ciencias Físicas, UNAM.

Since the proposal of the fluid mosaic model of the cell membrane by Singer and Nicolson (Singer and Nicolson 1972) our understanding of the role of it has changed considerably. From an inert matrix simply enclosing the cell, to a complex system where many biological processes occur, with the participation of the membrane, through its composition, structure and dynamics (Nicolson 2015; Troeira Henriques and Craik 2017; Desai and Miller 2018; Escribá and Nicolson 2014). It is now clear that the lipid bilayer is far from a homogeneous material, depending on its composition it can have domains with different properties, affecting the development of biological processes (Dos Santos et al. 2017). Recently Molecular Dynamics simulations have been used to study membranes at the molecular level, and certainly domains have been a sustained interest. In this talk we will be presenting MD studies of membrane systems as well as experimental results that help us to understand these formations and their biological relevance.

Constrained Dipole Moment Density Functional Theory for Charge Distributions in Force Fields for the Study of Molecular Fluids

Javier Carmona-Espíndola¹, Edgar Nuñez-Rojas¹, Valeria García-Melgarejo², José L. Gázquez², José Alejandro²

¹Departamento de Química, CONACYT-Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco 186, Ciudad de México, 09340, México.

²Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, Av. San Rafael Atlixco 186, México, Ciudad de México, 09340, México.

jcarmona_26@yahoo.com.mx

In this work, we present a new methodology to describe a system with a constrained dipole moment, CD-DFT. The self-consistent solution of this methodology leads to a unique density that minimizes the energy of the system for the pre-defined value of the dipole moment. With this methodology, we determined the atomic charges for the parametrization of force fields in classical molecular dynamics [1]. To this end, we implemented the atomic dipole moment corrected Hirshfeld population method, ADCH [2]. This method modifies the Hirshfeld charges so as to obtain the same molecular dipole moment associated with a given electronic distribution. The pre-defined values for the dipole moment in the self-consistent calculations are the ones that reproduce the dielectric constant of the corresponding fluid. The force field parameters thus obtained give a reasonable description of several properties like heats of vaporization, self-diffusion coefficients, shear viscosities, isothermal compressibilities and volumetric expansion coefficients of pure substances.

1. Salas, F. J.; Méndez-Maldonado, G. A.; Núñez-Rojas, E.; Aguilar-Pineda, G. E.; Domínguez, H.; Alejandro, J., Systematic Procedure To Parametrize Force Fields for Molecular Fluids. *J. Chem. Theory Comput.* **2015**, *11*, 683-693.
2. Lu, T.; Chen, F. W., Atomic dipole moment corrected Hirshfeld population method. *J. Theor. Comput. Chem.* **2012**, *11*, 163-183.

When drug–drug eutectic solids are formed instead drug–drug cocrystals: what to do?

Guadalupe Coyote-Dotor^a, Inés Fuentes-Noriega,^b Joelis Rodríguez Hernández, ^c Juan Manuel Germán-Acacio^a

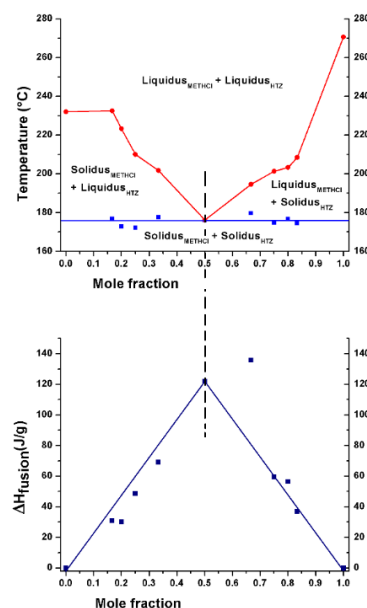
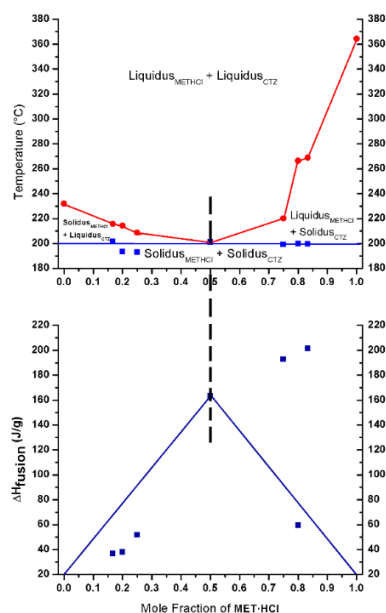
^a Red de Apoyo a la Investigación, Universidad Nacional Autónoma de México-CIC, Instituto Nacional de Ciencias Médicas y Nutrición SZ, C. P.14000, Ciudad de México, México.

^b Laboratorio de Biofarmacia, Departamento de Farmacia, Facultad de Química, UNAM.

^c Centro de Investigación en Química Aplicada (CIQA), Boulevard Enrique Reyna Hermosillo No. 140, Saltillo, Coahuila 25294, México

Abstract

In this work is described the formation by mechanochemical procedures of drug–drug solid forms containing metformin hydrochloride (MET·HCl) in the presence of thiazide diuretics: hydrochlorothiazide (HTZ) or chlorothiazide (CTZ). The thorough characterization indicates the formation of binary eutectic conglomerates, that we have denominated as drug–drug eutectic solids (DDESs). The DDESs were characterized by diverse techniques: thermal analysis (DSC and TGA), solid state NMR spectroscopy (ssNMR), Powder X-Ray Diffraction (PXRD) and Scanning Electron Microscopy/Energy Dispersive X-Ray Spectroscopy analysis (SEM/EDS). Intrinsic dissolution rate experiments demonstrated a slight enhancement in the % release of HTZ in the solid forms MET·HCl-HTZ 1:1 and 2:1 compared with pure drug. However, solid forms MET·HCl-CTZ 1:1, 1:2 or 2:1 showed a decrement in the % release of CTZ in the dissolution profiles.



TITLE

Aqueous solutions of methanol, ethanol and 1-propanol: numerical simulations of the liquid phase and liquid-vapor coexistence using refined molecular models

SPEAKER

Dr. Manuel Martínez Jiménez
Universidad Autónoma Metropolitana, Unidad Iztapalapa

ABSTRACT

Primary alcohols are organic compounds that belong to one of the most important solvent classes because of their practical applications. The aqueous solutions of these alcohols have been the subject of various theoretical and experimental studies, both in the liquid phase and in the liquid-vapor coexistence, providing mutually complementary information to understand the physical properties of these systems. However, in the case of numerical simulations, most of the previous works have used potential optimized only for the liquid phase of each component and partially incorrect simulation protocols, which motivate the review of the reported results.

In this talk I will present a set of analytical potentials for the aqueous solutions of methanol, ethanol and 1-propanol that were used in the study of the liquid and liquid-vapor phase, using classical molecular dynamics. The new models were optimized to reproduce the density, dielectric constant and surface tension of pure liquids at 298 K ($p = 1$ bar). I will discuss the differences with respect to the existing potentials and the predictive capacity of the new models in the liquid phase, in particular, the excesses of volumes and enthalpies of mixing. I will also show the characterization of the liquid-vapor interfaces by calculating density profiles, surface tension, angular orientations and electrostatic potentials, as a function of the molar composition of each alcohol. The importance of adequate treatment of long-range interactions and the finite size effects of the systems studied will also be discussed.

Low Hydroxylated Fullerenes: Stability, Thermal Behavior, and Vibrational Properties

M. V. Velarde-Salcedo^a, M. Gallo^b, and R. A. Guirado-Lopez^c

^aUniversidad Autónoma del Estado de México, Instituto Literario 100, CP 50000, Toluca

^bTecnologico Nacional de Mexico/ITCJ, Av. Tecnológico 1340, Cd. Juárez, Chihuahua 32500, Mexico

^cInstituto de Física “Manuel Sandoval Vallarta”, Universidad Autónoma de San Luis Potosí, Alvaro Obregon 64, San Luis Potosí, S.L.P. 78000, Mexico

Extensive density functional theory calculations dedicated to analyze the stability, thermal behavior, as well as the infrared and Raman spectra of low hydroxylated fullerenols C₆₀(OH)₁₂ are presented. It is found that the formation of local networks of hydrogenbonded OH groups plays a fundamental role in the stability of these complexes. The calculated dipole moments, polarizability values, optical gap, and Fukui functions of C₆₀(OH)₁₂ isomers strongly depend on the structure of the hydroxyl overlayer, thus being an important parameter to tune the material properties. DFT Born–Oppenheimer molecular dynamics calculations at T = 300 K reveal that aggregated forms of OH groups on the fullerene surface show an interesting dynamical behavior, characterized by a continuous proton-exchange process between neighboring hydroxyl molecules that modifies the structure and chemical nature of the molecular coating. From nudged elastic band studies analyzing OH diffusion on the C₆₀ surface, energy barriers opposing OH migration of ~1 eV are found. However, in the presence of surrounding H₂O species, a water-assisted diffusion process is obtained which can reduce the energy barriers to values as low as 0.25 eV. The comparison between experimental and calculated IR spectra of various C₆₀(OH)₁₂ isomers shows well-defined spectral features which can be helpful to identify the structure of these fullerene complexes. Finally, simulations of the wavelength-dependent Raman spectra of hydroxylated fullerenes reveals (i) that the intensities of the Raman active modes strongly depend on the excitation laser and (ii) the importance of the wavelength-dependent calculations to reveal precise features of different regions of the spectra (J. Phys. Chem. C 2018, 122, 13117–13129).

Dielectric behavior of water within a surfactant bilayer: a molecular dynamics study

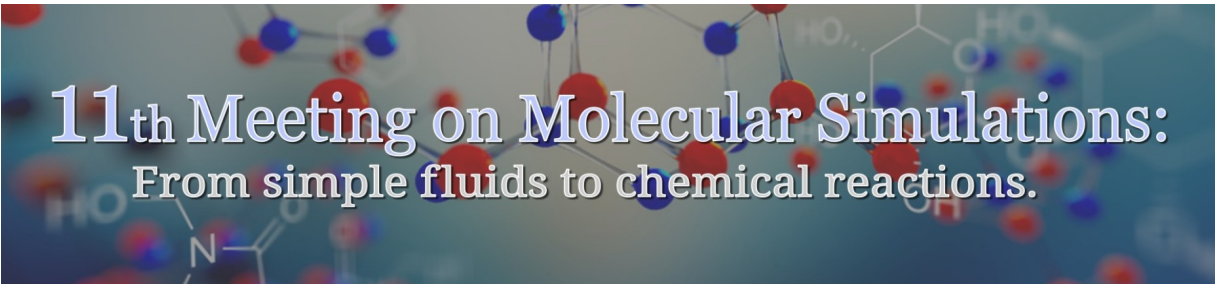
Minerva González Melchor, Efraín Meneses and Juan Francisco Rivas

Instituto de Física "Luis Rivera Terrazas", Benemérita Universidad Autónoma de Puebla

Apartado Postal J-48, Puebla, 72570, México

minerva@ifuap.buap.mx

Understanding the dielectric behavior of water confined within a surfactant bilayer is essential in the description of different physicochemical processes in biological systems, drug design and enhanced oil recovery, among others. Although extensive work has been done for surfactant and lipid bilayers, less attention has been paid to the dielectric behavior of water confined in it. From the point of view of simulations there is a standard procedure to evaluate the static dielectric constant of a fluid in one-phase simulations, however there are limited attempts to determine the dielectric behavior of water in bilayer geometries. In this work we study the dielectric behavior of water confined between two layers of surfactant. We use four models that have been useful in the description of different properties of liquid water in a wide range of thermodynamic conditions but predict different values of static dielectric constant. The surfactant molecules are described using models proposed in the literature. Our results are discussed in terms of the evaluation of the static dielectric constant of water and structural properties in the bilayer for the SPC/E, TIP4P/2005, TIP4Q and SPCepsilon models. These results are necessary to lay the foundations for a better dielectric characterization of the water contained in films and open the possibility to propose methods that allow the evaluation of these properties when molecular simulations are applied.



11th Meeting on Molecular Simulations: From simple fluids to chemical reactions.

Líquidos iónicos en los procesos de desulfuración y desnitrogenación de hidrocarburos.

N.V. Likhanova¹, I.V. Lijanov²

¹*Instituto Mexicano del Petróleo, Eje Central Lázaro Cardenas Norte, 152, col. San Bartolo Atepehuacan, 07730, CDMX*

²*Instituto Politécnico Nacional, CIITEC, Cerrada Cecati S/N, Colonia Santa Catarina de Azcapotzalco, CP 02250, CDMX*

Según las nuevas normas del medio ambiente de la Unión Europea y los Estados Unidos de América, establecidas en 2010, los productores de diésel tienen que disminuir la cantidad de azufre para alcanzar niveles no superiores a 15 partes por millón. En nuestro caso, los PEMEX Refinación aceptó este compromiso con el fin de producir y distribuir diésel con contenido ultra bajo azufre (DUBA) que cumple con todos los requisitos de la legislación ambiental bajo los estándares internacionales.

El método clásico utilizado hoy en las refinerías para la desulfuración de hidrocarburos del petróleo es la hidrodesulfuración catalítica a altas presiones y temperaturas (proceso HDS). Sin embargo, dicho proceso es muy costoso; necesita condiciones de operación drásticas, así como el uso de catalizadores de metales nobles que se envenenan con bastante rapidez. Es cierto que HDS es un proceso eficiente para la reducción de compuestos alifáticos de azufre, pero no es tan efectivo en la reducción de compuestos aromáticos de azufre, especialmente en el caso de aceites mexicanos pesados. Los cortes de refinería generalmente contienen un bajo nivel de compuestos a base de nitrógeno (0.1% a 2%), pero el contenido de nitrógeno aumenta con el aumento del punto de ebullición de una fracción de aceite particular. Los compuestos a base de nitrógeno se consideran inhibidores fuertes y venenos para los catalizadores de hidrodesulfuración.

Los líquidos iónicos (LIs) se conocen desde hace más de 30 años, pero su aplicación en diferentes procesos industriales se inició hace solo unos 10 años. Se usan como solventes y catalizadores en reacciones de alquilación, polimerización, Diels-Alder, en electroquímica, pero su uso más interesante es como solvente en la extracción de CO₂, compuestos aromáticos y de azufre de las mezclas de hidrocarburos. La variedad de LIs depende de los tipos de cationes y aniones utilizados. Como hay innumerables combinaciones, esto los hace interesantes para los procesos de extracción porque siempre podemos encontrar un LI adecuado para cualquier sistema de extracción individual. Recientemente, se han estudiado nuevos procesos para eliminar azufre y nitrógeno de las corrientes de refinería, incluido el uso de líquidos iónicos como extractante.

En nuestros trabajos, evaluamos los LIs con los cationes heterocíclicos basados en imidazolio, piridinio y alquilamonio y distintos aniones para los procesos de desulfuración y desnitrogenación de hidrocarburos.

Correo-e: nvictoro@imp.mx

Interfacial strain defines the self-organization of epitaxial MoO₂ flakes and porous films on sapphire: experiments and modelling

O. de Melo,^{1,2,3} V. Torres-Costa,² Y. González,^{2,4} A. Ruediger,⁴ C. de Melo,⁵ J. Ghanbaja,⁵ D. Horwat,⁵ A. Escobosa,⁶ O. Concepción,^{2,6,1} G. Santana,³ E. Ramos³

¹Physics Faculty, University of Havana, 10400 La Habana, Cuba

²Departamento de Física Aplicada, Universidad Autónoma de Madrid. Cantoblanco 28049, Madrid, Spain

³Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Cd. Universitaria, A.P. 70-360, Coyoacán 04510, México D. F.

⁴Institut National de la recherche scientifique, Centre Énergie, Matériaux, Télécommunications, 1650 Boulevard Lionel-Boulet, Varennes, Québec, J3X 1S2, Canada

⁵Institut Jean Lamour, Université de Lorraine, UMR 7198, Nancy, F-54000, France

⁶Sección de Electrónica del Estado Sólido, Departamento de Ingeniería Eléctrica, CINVESTAV, IPN, Mexico

Abstract. The epitaxy of MoO₂ on c-plane sapphire substrates is examined. A theoretical approach, based on density functional theory calculations of the strain energy, allowed to predict the preferred layer/substrate epitaxial relationships. To test the results of these calculations, MoO₂/(001) Al₂O₃ heterostructures were grown using the chemically driven isothermal close space vapour transport technique. At the early stage of the growth, two kinds of morphologies were obtained, with the same growth parameters: lying and standing flakes. X-ray diffraction, scanning and transmission electron microscopy, transmission electron diffraction as well as optical microscopy and Raman spectroscopy, allowed to determine the composition, the morphology, the layer/substrate epitaxial relationship and the orientation with respect to the substrate for both kind of morphologies. Observed epitaxial relationships coincide with those predicted as the most favourable ones in terms of strain energy, according DFT estimations. For thicker films, the standing flakes evolve to form a layer composed by coalescent epitaxial flakes in the form of an epitaxial porous layer. So, the interfacial strain between the sapphire substrate and MoO₂ enables a self-organization at nanometer to micron scales, depending on deposition conditions, between the flakes at early deposition stages and within porous films obtained at later deposition stages.

1 Presently at: MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, the Netherlands.

Aplicación de Líquidos Iónicos derivados de imidazol en la extracción de compuestos fenólicos a partir de productos naturales.

Zaira Domínguez
Unidad de Servicios de Apoyo en Resolución Analítica
Universidad Veracruzana

Los líquidos iónicos (LIs) son reconocidos como una nueva clase de disolventes verdes. Debido a sus características únicas, los LIs han encontrado aplicaciones, en síntesis, catálisis y procesos de extracción. Dado que pueden disolver celulosa, permiten un fácil acceso para extraer compuestos bioactivos con valor agregado a partir de material vegetal. Tal es el caso de los compuestos fenólicos. No obstante, compuestos de este tipo también están presentes en otro tipo de matrices de origen natural, como es el caso de los propóleos. A continuación, se presentan los resultados de la extracción de los principales compuestos fenólicos presentes en productos naturales, tales como propóleos y residuos de café, particularmente los conocidos como café gastado, empleando soluciones acuosas de LIs derivados de imidazol y otras tecnologías verdes como ultrasonido y microondas.