Methanol-water mixtures: a systematic study of liquid phase using non-polarizable models

Manuel Martínez Jiménez[a,b], Humberto Saint-Martin Posada[b]
[a]Posgrado en Ciencias Físicas, UNAM; México [b] Instituto de Ciencias Físicas, UNAM; México
mm_ximenez@yahoo.com

Molecular dynamics simulations are used to study thermodynamic, dynamic and structural properties of the water-methanol mixtures as a function of the methanol molar fraction. Unlike previous studies in recent literature, in this work we use molecular models which reproduce the experimental value of dielectric constant for each liquid (T = 298.15 K y p = 1 bar). These analytical potentials are the TIP4P/ε[1] model for water, whereas for methanol we use the model of Salas, J. and Alejandre, J.[2] and a new parameterization which improves the description of the binary mixtures.

[1] Fuentes-Azcatl, R.; Alejandre, J. Non-polarizable force field of water based on the dielectric constant: TIP4P/ε. J. Phys. Chem. B, **2014**, 118 (5), 1263-1272.

[2] Salas, F.J.; Alejandre, J. Systematic procedure to parametrize force fields for molecular fluids. J. Chem. Theory Comput., **2015**, 11 (2), 683-693.

LATERAL HETEROGENEITY OF CHOLESTEROL ON BINARY LIPID MIXTURES OF POPC/CHOL: A MOLECULAR DYNAMICS STUDY

Fernando Favela-Rosales[1,2], Arturo Galván-Hernández[1], Jorge Hernández-Cobos[1] and Iván Ortega-Blake[1]

[1]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Av Universidad s/n, Cuernavaca, Morelos, 62251, México.
[2]Departamento de Investigación, Instituto Tecnológico Superior Zacatecas Occidente, Av. Tecnológico No. 2000, Sombrerete, Zacacatecas, 99100, México.

Phase diagrams on ternary and quaternary lipid mixtures showing the existence of liquid-disordered (ld), liquid-ordered (lo) and a mixed phase (ld+lo) are now well established. Although the ld+lo is generally accepted for binary mixtures of cholesterol and phospholipids with saturated acyl chains, the existence of a phase separation in mixtures of cholesterol with phospholipids that have one saturated and one unsaturated acyl chain is not universally accepted. There are reports of a phase diagram on the mixtures POPC/Chol and POPC/Erg and nystatin activity co-related to this purported phase diagram; with a maximal activity appearing in the mixed phase. In a recent work we presented a Molecular Dynamics (MD) study of a POPC membrane with different cholesterol concentrations along the phase diagram and computed the order parameters binned in the xy-plane as well as the cholesterol density. The results support the existence of a lateral heterogeneity of cholesterol, present mainly in the mixed phase. Here we extend the previous study to consider also membrane thickness as well as the evolution of these distributions along a μs of simulation. We observed structures that support the idea of cholesterol lateral heterogeneity is present in this binary mixture. The MD simulations allowed us to advance in the understanding of the molecular structure changes resulting from phase differences. Funding: DGAPA-PAPIIT-RG100416 and ITSZO.

Effect of H-bonds in the rheological behavior of the ionic liquid 1-butyl-3-methylimidazolium bis(trifluromethylsulfonyl)imide [bmim][Tf_2N] by Molecular Dynamics

E. G. Blanco-Díaz, E. O. Castrejón-González

Department of Chemical Engineering, Instituto Tecnológico de Celaya, Celaya Gto., 38010, México

Abstract

Ionic liquids (ILs) are molten salts at room temperature with a pair of ions: cation and anion. In recent years the study of this compounds has grown in the academic and industrial communities due to its properties[1,2]. Nowadays, there are lack of information about ILs in both bulk behavior and molecular structures. In order to deepen in the understanding of i) the IL interactions, ii) the H-bonds and iii) the structure generated by 1-butyl-3-methylimidazolium cation and bis(trifluromethylsulfonyl)imide anion ([bmim][Tf_2N]), we have carried out a Molecular Dynamics study. An H-bonding [C-H···O] analysis of [bmim][Tf_2N] has been made under the distance and energy criteria of weak H-bond (see Fig. 1-a). Furthermore, it was determined the interaction energy and number of H···O interactions with both Equilibrium Molecular Dynamics (EMD) and Non-Equilibrium Molecular Dynamics (NEMD). The rheological behavior of [bmim][Tf_2N] at 298.15 K has been calculated in a NVT ensemble together with SLLOD equations of motion in NEMD. The effect of H-bonds in the viscosity is associated with the decrease of interactions cation-anion while shear rate is increasing (Fig. 1-b).

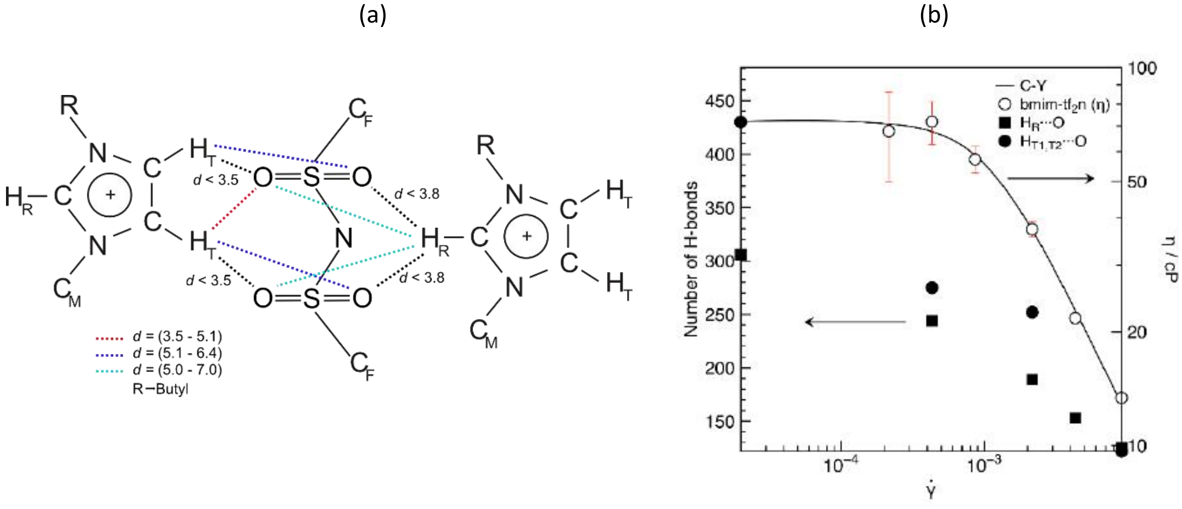
(a) (b)

Figure 1. Schematic representation of (a) both hydrogen bonds and large interactions on cations and anions, and (b) connection between viscosity and H-bonds vs $\dot{\gamma}$.

1. J. S. Wilkes, P. Wasserscheid and T. Welton. Ionic Liquids in Synthesis. Introduction. *Wiley-VCH*, 2008.
2. M. Deetlefs, M. Fanselow and K. R. Seddon. Ionic liquids: the view from mount improbable. RSC Adv., 6: 4280-4288, 2016.

Absorption of Benzene by Different Solvents.

Hugo M. Flores-Ruiz[a,b], Edgar Nuñez-Rojas[b] and José Alejandre[b]

[a]Departamento de Ingeniería, Universidad Autónoma del Estado de Hidalgo, campus Ciudad Sahagún. Colectivos Dina, zona industrial, 43970, Ciudad Sahagún, Hidalgo.
Email: hugomarcelofr@gmail.com

[a,b]Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa. Av. San Rafael Atlixco 186, Col. Vicentina, 09340, México Distrito Federal, México.

The presence of aromatic compounds in the gasoline is a serious and current problem. Carcinogenicity of these compounds has been demonstrated and therefore there exists the need to control the composition of such compounds. Typical separation methods like distillation present problems due to the volatile nature of the organic compounds. An alternative solution has been absorbing aromatic compounds by means of solvents with affinity with these molecules (Solvent extraction). Such solvents must have special features, they have to present solubility with aromatic compounds and at the same time they have to be polar, so that they do not mix with aliphatic hydrocarbons. Molecular Dynamics simulations of the absorption of benzene in both polar solvents and ionic liquids were carried out from a bezene/dodecane/solvent ternary mixture. Benzene absorbed was mixed with dodecane, this mixture emulated the gasoline with aromatic compounds. Results, based on density profiles analysis, showed that solvents which structure is based on the pyrrol functional group presented a good absorption and this is in an excellent agreement with experiments. On the other hand, it was found that ionic liquids with a ring containing two nitrogen atoms did not show affinity with benzene. This kind of absorption has been barely studied by molecular simulations before and it was found that with force field interaction parameters chosen it was possible to characterize the process as it has been observed experimentally.

Cluster Evolution in a Dissipative Soft System

Caty L. Morales-Martínez[1] and Rodrigo Sánchez [2*]

[1]Facultad de Ingeniería Civil, Universidad Veracruzana, Xalapa C.P. 91000, Veracruz.

[2]Departamento de Física, Universidad Autónoma Metropolitana Unidad Iztapalapa. Av.
San Rafael Atlixco 186, Col. Vicentina C.P. 09340, Ciudad de México.

The evolution of clusters in a soft granular submonolayer is examined [1]. Their final state is characterized in terms of the fractal dimension, typical cluster size and the mean number of nearest neighbours. Their evolution towards this state can be understood by considering dissipation and a Yukawa repulsion with time-dependent truncation. This approach is of potential interest for understanding other dissipative soft systems. The relationship found between cluster size and the number of nearest neighbours can be explained assuming the latter varies only due to the incorporation of new constituents. This assumption is likely applicable to numerous other statistical systems, making these results of interest well beyond the particular system examined.

References

[1] C. L. Morales-Martínez and R. Sánchez. Manuscript accepted by *J. Stat. Mech. Theor. Exp.*

[*] Author to whom correspondence should be addressed (rodrsanchez@xanum.uam.mx).

Thermodynamic properties of triangle-well fluids in two dimensions: MC and MD simulations

Yuri Reyes[1], Mariana Bárcenas[2], Gerardo Odriozola[3], Pedro Orea[4]

1 Departamento de Recursos de la Tierra, División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana Unidad Lerma.

2 División de Ingeniería Química y Bioquímica, Teconológico de Estudios Superiores de Ecatapec.

3 Área de Física de Procesos Irreversibles, División de Ciencias Básicas e Ingeniería, Autónoma Metropolitana Unidad Azcapotzalco.

4 Dirección de Investigación en Transformación de Hidrocarburos, Instituto Mexicano del Petróleo.

With the aim of providing complementary data of the thermodynamics properties of the triangular well potential, the vapor/liquid phase diagrams for such potential with different interaction ranges were calculated in two dimensions by Monte Carlo and molecular dynamics simulations; also, the vapor/liquid interfacial tension was calculated. As reported for other interaction potentials, it was observed that the reduction of the dimensionality makes the phase diagram to shrink. Finally, with the aid of reported data for the same potential in three dimensions, it was observed that this potential does not follow the principle of corresponding states.

References

Y. Reyes, M. Bárcenas, G. Odriozola, P. Orea. *J. Chem. Phys.* **2016**, 145, 174505.

POSSIBLE RAPAMICINE, FK-506 AND FKBP12 INTERACTION SITES ABOUT THE TMEM16A CHANNEL ACTIVITY

Gloria Arlette Méndez Maldonado[1], Jose Juan de Jesus Perez[2], Jorge Arreola[2].
[1] Cátedra CONACyT- Facultad de Medicina,UASLP, [2] Instituto de Física, UASLP

The TMEM16A protein is a calcium activated chloride channel (CaCC). It is present in various sensory cells, including: olfactory neurons, photosensitive receptors and dorsal root ganglia. They are involved in the regulation of epithelial transport, smooth muscle contraction, neuronal and cardiac excitability, and sensory transduction. Rapamycin and FK-506 are structurally related macrolide antibiotics. The effects as immunosuppressants are well recognuzed and are known to be mediated by their interaction with the FKBP12 immunophilin. In this work, using computational Docking techniques, the possible mechanisms by which rapamycin, FK-506 and FKBP12 modulate the TMEM16A channel in silico will be analyzed. Initially, we considered the possibility of a direct interaction between rapamycin and FK-506 with TMEM16. However, our results suggest that the effects exerted by both immunosuppressants are mediated by the FK-BP12 binding protein, as has been shown to occur in the immune system.

The line tension of an ionic fluid

M. R. Eustaquio-Armenta, G. A. Méndez-Maldonado, M. González-Melchor
Instituto de física “Ing. Luis Rivera Terrazas”, BUAP, Apdo. Postal J-48, Puebla, Pue. C.P. 72570

We carried out classical molecular dynamics simulations in the canonical ensemble (NVT) to calculate the line tension associated to the liquid-vapor interface of a mixture of equally charged ions modeled through the soft primitive model. We derived the two dimensional pressure tensor components needed in the calculation. The Ewald parameters, cutoff radius and interfacial length were chosen to make sure that the line tension values were free from artifacts. We found a decreasing behavior of the line tension as temperature increases.

Discrete Perturbation Theory for Mie Potentials.

I. M. Zerón (1), L. A. Padilla (1), F. Gámez (2), J. Torres–Arenas (1), A. L. Benavides (1).

(1) División de Ciencias e Ingenierías, Universidad de Guanajuato, Loma del Bosque 103, Colonia Lomas del Campestre, C.P. 37150. León, Guanajuato, México.

(2) Departamento de Sistemas Físicos, Químicos y Naturales, Universidad Pablo de Olavide, 41013 Sevilla, España.

We present an equation of state for Mie (a, b) potentials [1] based on the Discrete Perturbation Theory (DPT)[2]. Using a discrete version of the intermolecular potential given as a sequence of square shoulder and/or square wells, an analytic expression for the Helmholtz free energy can be obtained as a function of the density and temperature. Some illustrative cases with different intermolecular parameters (a, b) are shown. The vapor-liquid phase diagram, internal energies and pressures are compared with own simulation data and with data from the literature [3-7] obtaining a good agreement. It is shown that from the theoretical vapor-liquid equilibrium curves for Mie potentials a Corresponding States Principle is satisfied.

References

[1] G. Mie, *Annalen der Physik.* 316, 657-697, **1903**.

[2] A. L. Benavides, A. Gil-Villegas, *Molecular Physics.* 97, 1225-1232, **1999**.

[3] H. Okumura, F. Yonezawa, *The Journal of Chemical Physics.* 113, 9162-9168, **2000**.

[4] P. Orea, Y. Reyes-Mercado, Y. Duda, *Physics Letters A.* 372, 7024-7027, **2008**.

[5] N. S. Ramrattan, C. Avendaño, E. A. Müller, A. Galindo, *Molecular Physics.* 113, 932-947, **2015**.

[6] A. Trokhymchuk and J. Alejandre, *The Journal of Chemical Physics*, 111, 8510-8523, **1999**.

[7] J. K. Johnson, J. A. Zollweg, K. E. Gubbins, *Molecular Physics.* 78, 591-618, **1993**.

Discrete Perturbation Theory for Mie Potentials.

I. M. Zerón (1), L. A. Padilla (1), F. Gámez (2), J. Torres–Arenas (1), A. L. Benavides (1).

(1) División de Ciencias e Ingenierías, Universidad de Guanajuato, Loma del Bosque 103, Colonia Lomas del Campestre, C.P. 37150. León, Guanajuato, México.

(2) Departamento de Sistemas Físicos, Químicos y Naturales, Universidad Pablo de Olavide, 41013 Sevilla, España.

We present an equation of state for Mie (a, b) potentials [1] based on the Discrete Perturbation Theory (DPT)[2]. Using a discrete version of the intermolecular potential given as a sequence of square shoulder and/or square wells, an analytic expression for the Helmholtz free energy can be obtained as a function of the density and temperature. Some illustrative cases with different intermolecular parameters (a, b) are shown. The vapor-liquid phase diagram, internal energies and pressures are compared with own simulation data and with data from the literature [3-7] obtaining a good agreement. It is shown that from the theoretical vapor-liquid equilibrium curves for Mie potentials a Corresponding States Principle is satisfied.

References

[1] G. Mie, *Annalen der Physik.* 316, 657-697, **1903**.

[2] A. L. Benavides, A. Gil-Villegas, *Molecular Physics.* 97, 1225-1232, **1999**.

[3] H. Okumura, F. Yonezawa, *The Journal of Chemical Physics.* 113, 9162-9168, **2000**.

[4] P. Orea, Y. Reyes-Mercado, Y. Duda, *Physics Letters A.* 372, 7024-7027, **2008**.

[5] N. S. Ramrattan, C. Avendaño, E. A. Müller, A. Galindo, *Molecular Physics.* 113, 932-947, **2015**.

[6] A. Trokhymchuk and J. Alejandre, *The Journal of Chemical Physics*, 111, 8510-8523, **1999**.

[7] J. K. Johnson, J. A. Zollweg, K. E. Gubbins, *Molecular Physics.* 78, 591-618, **1993**.

INTERACTION ENERGY THROUGH AB INITIO CALCULATIONS FOR THE α-QUARTZ/NICKEL SYSTEM

Sergio Damián Vázquez (1), Juan Francisco Javier Alvarado (2), Edgar Omar Castrejón González (3)
(1) Departamento de Ingeniería Química, Instituto Tecnológico de Celaya, Celaya, Guanajuato, 38010, MEXICO.
sergio.vaquez@iqcelaya.itc.mx
(2) Departamento de Ingeniería Química, Instituto Tecnológico de Celaya, Celaya, Guanajuato, 38010, MEXICO.
javier@iqcelaya.itc.mx
(3) Departamento de Ingeniería Química, Instituto Tecnológico de Celaya, Celaya, Guanajuato, 38010, MEXICO.
omar@iqcelaya.itc.mx

Carbon nanotubes (CNTs) are widely studied due to their excellent electrical, mechanical, and thermal properties, besides being able to combine with other elements to attain specific properties [1]. There are several methods for the synthesis of CNTs, such as laser ablation, arc discharge and Chemical Vapor Deposition [2]. The last, is known as the most efficient method for large-scale production of CNTs, which involves a carbon source (CH_4, C_2H_4, C_6H_6) catalyzed by metal nanoparticles (Fe, Co, Ni) on a substrate (SiO_2, Al_2O_3) [3]. The most common substrate used nowadays is the a-Quartz, which is the most stable crystal structure of SiO_2 at atmospheric conditions [4]. However, one of the main issues when the CNTs are growing is to control the nanotube diameter, which is related to the size of the catalytic nanoparticle. Thus, molecular dynamics is an excellent tool to investigate this kind of interactions crystal/metal. Energy of interaction (adsorption) is the first calculation to obtain an interatomic potential in order to perform large-scale molecular dynamics. In this case, we have studied the interaction a-Quartz/Nickel that is observed in Chemical Vapor Deposition (CVD) processes to synthesize carbon nanotubes. To obtain the *Ab Initio* training set, all the systems were optimized with VASP (Vienna Ab Initio Simulation Package) [5] using the projector augmented wave method (PAW) and Perdew-Burker-Ernzerhof (PBE), with a high precision.

References

[1] J.-C. Charlier, X. Blase and S. Roche, *Rev. Mod. Phys.*, 2007, **79**, 677-732.
[2] I. Bustero, G. Ainara, O. Isabel, M. Roberto, R. Inés and A. Amaya, *Microchimica Acta*, 2006, **152**, 239-247.
[3] L. Vanyorek, D. Loche, H. Katona, M. F. Casula, A. Corrias, Z. Knya, Kukovecz and I. Kiricsi, *The Journal of Physical Chemistry C*, 2011, **115**, 5894-5902.
[4] T.-R. Louise Levien, Charles T. Prewitt and D. J. Weidner, *American Mineralogist*, 1980, **65**, 920-930.
[5] J. Hafner, *Journal of Computational Chemistry*, 2008, **29**, 2044-2078.

Exploring the conformational space of variants of Bcl-2 protein: Dynamical contributions of the Flexible Long Domain and Transmembranal region

Caro-Gómez Luis A. (1), Vique-Sánchez José L (1), Rosas-Trigueros Jorge L. (2), Mixcoha-Hernández Edgar (3), Benítez-Cardoza Claudia G (1). and Zamorano-Carrillo Absalom (1).

(1). Laboratorio de Bioquímica y Biofísica Computacional, ENMH, Instituto Politécnico Nacional. México D.F. (2) Laboratorio Transdisciplinario de Sistemas Evolutivos, ESCOM, Instituto Politécnico Nacional. México D.F. (3) Instituto Nacional de Psiquiatría RFM México D.F. Email: plrbilo@gmail.com, azamorano@ipn.mx

All multicellular organisms must have an exquisite regulation of their cell mass turnover during all their lifespan to avoid a variety of severe health disorders (1). Apoptosis is the most common programmed cell death process in mammals. Members of the Bcl-2 protein family flawlessly regulate the apoptotic process through interactions with several proteins including members of the same family (2). Bcl-2 is the archetypical member of the family. This protein is characterized by an intrinsically disordered region depicted as “flexible loop domain” (FLD), and a transmembranal (TM) region that anchors mitochondrial external membrane (3). Here we performed a comparative analysis of the archetypical member of the family (Bcl-2) and one naturally occurring protein (Bcl-2A1) that lacks FLD as well as two artificial constructs lacking the C-terminal domain (Bcl-2ΔTM and Bcl-2A1ΔTM). We describe, at an atomistic level the conformational changes of each construct that might be associated with the function of these proteins. We have found that both FLD and TM regions stabilize Bcl-2 proteins. When both domains are present, they show a synergistic stabilizing effect. These results have important implications for understanding interactions between members of the Bcl-2 family and might be useful in rational drug design.

1.P. E. Czabotar, G. Lessene, A. Strasser, and J. M. Adams, (2014) “Control of apoptosis by the BCL-2 protein family: implications for physiology and therapy.,” Nat. Rev. Mol. Cell Biol.

2.C. Borner, (2003) “The Bcl-2 protein family: Sensors and checkpoints for life-or-death decisions,” Mol. Immunol.

3.Ilizaliturri-Flores, J. Correa-Basurto, M. Bello, J. L. Rosas-Trigueros, B. Zamora-López, C. G. Benítez-Cardoza, and A. Zamorano-Carrillo, (2016) “Mapping the intrinsically disordered properties of the flexible loop domain of Bcl-2: a molecular dynamics simulation study,” J. Mol. Model.

Viscosity Calculation using Equilibrium Molecular Dynamics Simulations for the [C_4mim][PF_6] ionic liquid.

Joel Sánchez-Badillo[1], Marco Gallo[2*], Ricardo Guirado[3], Raúl González-García[1], Albero Duarte-Moller[4]

[1] 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.
[2] Tecnológico Nacional de México, Av. Tecnológico 1340, Chih, 32500. *correo electrónico mgallo@itcj.edu.mx
[3] Instituto de Física, Universidad Autónoma de San Luis Potosí (UASLP), Av. Manuel Nava No. 6, Zona Universitaria, San Luis Potosí, S.L.P. 78210, México.
[4] Centro de Investigación en Materiales Avanzados, Miguel de Cervantes 120, Complejo Industrial Chihuahua, Chih. México. C.P. 31136.

Abstract

In this work we calculated the shear viscosity for the [C_4mim] [PF_6] ionic liquid by using the Green-Kubo equation with block time-origin analysis[1] and equilibrium molecular dynamics simulations in the *NVT* ensemble at 350 K; Several analysis were carried in order to determine the appropriate equilibration and production times to ensure a diffusive regime[2,3], also the following variables were determined to obtained robust viscosity calculations: length of simulation time (t_d), window width (t_w), spacing between windows (t_s),[1] and the number of terms in the pressure tensor (P_{ij}) and their combination needed, in order to obtain robust results for the ionic liquid viscosity.[1,4-9]

The calculation of the shear viscosity is a difficult task because of the sluggish dynamic behavior of the ionic liquids.[2,9] The first step to obtain appropriate viscosity calculations is to verify that the [C_4mim][PF_6] lies on the diffusive regime,[2,3] determined by the $\alpha^2(t)$[2,3] and $\beta(t)$,[2] metrics; The diffusive regime is promoted using equilibrium simulations with more than 50 ns with an *all-atom* force field and high temperatures. Also is important to determine the necessary components of the pressure tensor and their combination for reliable statistics.[8] Next, the calculation of the shear viscosity is performed using the block time-origin analysis[1] to obtain a robust behavior for the pressure-correlation function[9] and finally we performed an average over 10-20 independent molecular dynamics trajectories similar to Maginn et al.[10] The molecular simulations in this work used an *all-atom* force field developed by Gallo et al.[11].

References

[1] Nevins, D.; Spera, J. Accurate Computation of Shear Viscosity from Equilibrium Molecular Dynamics Simulations. *Mol. Simulat.* **2007,** *33*, 1261-1266.

[2] Kelkar, M. S.; Maginn, E. J. Effect of Temperature and Water Content on the Shear Viscosity of the Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethanesulfonyl)imide As Studied by Atomistic Simulations. *J. Phys. Chem. B* **2007,** *111*, 4867-4876.

[3] Mondal, A.; Balasubramanian, S. A Refined All-Atom Potential for Imidazolium-Based Room Temperature Ionic Liquids: Acetate, Dicyanamide, and Thiocyanate Anions. *J. Phys. Chem. B* **2015,** *119*, 11041–11051.

[4] Liu, H.; Maginn, E. A Molecular Dynamics Investigation of the Structural and Dynamic Properties of the Ionic Liquid 1-n-Butyl-3-methylimidazolium Bis(trifluoromethanesulfonyl)imide. *J. Chem. Phys.* **2011,** *135*, 124507.

[5] González, M. A.; Abascal, J. L. F. The Shear Viscosity of Rigid Water Models. *J. Chem. Phys.* **2010,** *132*, 096101.

[6] Van-Oanh, N.-T.; Houriez, C.; Rousseau, B. Viscosity of the 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquid from Equilibrium and Nonequilibrium Molecular Dynamics. Phys. Chem. Chem. Phys. **2010,** *12*, 930–936.

[7] Bedrov, D.; Smith, G. D.; Sewell, T. D. Temperature-Dependent Shear Viscosity Coefficient of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX): A Molecular Dynamics Simulation Study. *J. Chem. Phys.* **2000,** *112*, 7203-7208.

[8] Rey-Castro, C.; Vega, L. F. Transport Properties of the Ionic Liquid 1-Ethyl-3-Methylimidazolium Chloride from Equilibrium Molecular Dynamics Simulation. The Effect of Temperature. *J. Phys. Chem. B* **2006,** *110*, 14426-14435.

[9] Mondal, A.; Balasubramanian, S. A Molecular Dynamics Study of Collective Transport Properties of Imidazolium-Based Room-Temperature Ionic Liquids. *J. Chem. Eng. Data* **2014,** *59*, 3061–3068.

[10] Zhang, Y.; Otani, A.; Maginn, E. J. Reliable Viscosity Calculation from Equilibrium Molecular Dynamics Simulations: A Time Decomposition Method. *J. Chem. Theory Comput.* **2015,** *11*, 3537–3546.

[11] Gallo, M et al., in preparation for publication.

“Un nuevo modelo del Oregonador”

[a]Jesús Andrés Arzola Flores
[a]Laboratorio de Energía. Instituto de Física. Benemérita Universidad Autónoma de Puebla.
Av. San Claudio S/N. Col. San Manuel. Puebla, Pue. C.P 72590

Resumen

La reacción de Belousov-Zhabotinsky (BZ) ha sido muy estudiada debido a su analogía con mecanismos de retroalimentación química presentes en la fisiología humana [1]. Muchos han sido los esfuerzos por entender la dinámica de dicha reacción química mediante modelos matemáticos de ecuaciones diferenciales ordinarias no lineales [2,3,4]. Sin embargo, el mecanismo de reacción no ha sido del todo explicado, puesto que los modelos planteados únicamente describen un comportamiento parcial de la reacción. En el presente trabajo se obtiene una mejor aproximación matemática para explicar el comportamiento no lineal de la reacción de Belousov-Zhabotinsky. Un modelo más robusto de la dinámica de la reacción BZ serviría para entender detalladamente el mecanismo de reacción así como sus múltiples aplicaciones. Una aplicación de la reacción BZ podría ser en el área de la Medicina, debido a que dicha reacción podría emplearse como sensor químico, el cual podría detectar especies químicas como la glucosa, ácido úrico, colesterol, etc, debido a que la presencia de una especie química extraña en la reacción BZ podría provocar una variación en la amplitud y periodo de las oscilaciones químicas.

Bibliografía

[1] R Curi. Arq Bras Endocrinol Metab. 47, 135, (2003).
[2] R.J.Field and R.M.Noyes, J.Chem.Phys. 60, 1877 (1974).
[3] R.J.Field,E.Koros,R.M.Noyes, JACS 94,8649 (1972).
[4] R.J.Field, R.M.Noyes, Nature 237,390 (1972).

SURFACE TENSION OF NaCl IN WATER

Gabriela Y. Espejo Villaldama (1), Liliana Guerrero Turrubiates (1), Gabriel E. Torres Ramírez (1).

(1) *Departamento de Ciencias Biológicas y de la Salud. Universidad Autónoma Metropolitana-Xochimilco. Calzada del Hueso 1100, Coyoacán, Villa Quietud, 04960, Ciudad de México, México.*

The biochemical significance of the NaCl-H_2O solution In living beings, coupled to its commercial and industrial importance, raises numerous questions of its behavior under different conditions; facing the difficulty of multiple experimentation with numerous variables, chemistry has found in molecular dynamics simulations a promising scope to understand and predict the physical and chemical properties.

Two proposals for theoretical-computational models were analyzed for the description of NaCl in aqueous solution: NaCl/ε, a parameterized force field that optimizes the radial particle-particle interaction, involving the Lennard-Jones and Coulomb potentials, so that the model can adequately reproduce the experimental data and the SPC/ε model that defines water as a non-polarizable rigid molecule where the intermolecular force field between two water molecules is also led by the Lennard-Jones potential and Coulomb interactions.

The main objective was to analyze together the surface tension in correlation with experimental data, which is the amount of energy needed to stretch or increase the surface area of a liquid per unit area, involving intermolecular forces, therefore, surface interaction is directly proportional to the size of those forces. The methodology used for correlation consisted in the representation of the molecular dynamics simulation with GROMACS, were the motion equations were solved using the Leap-frog algorithm in the overall NPT conditions: pressure of 1 bar, temperature of 293 K in a system 1024 NaCl pairs. The surface tension of a planar interface was calculated from the mechanical definition of γ. The results obtained were graphed as follows: the change in the relative surface tension in H_2O against molar concentration, comparing the data obtained from the NaCl/ε + SPC/ε model and the experimental data, showing a close reproduction of experimental data, hence it can by inflicted that the parameterization of NaCl/ε and SPC/ε makes this model able to replicate the experimental data through molecular dynamics simulations.

References

[1] R. Fuentes-Azcatl, M. C. Barbosa. (febrero 18,2016). *Sodium Chloride, NaCl/ε: New Force Field*. J. Phys. Chem. B, 120 (9), pp 2460–2470.

ABSTRACT SUBMISSION

Rational search for a compound that selectively inhibits the triose phosphate isomerase from *Trichomonas vaginalis*.

Navarro Salazar AR[1] Vique Sanchez JL[1], Caro Gómez LA[1] Brieba Luis[2], Arturo Rojo[3], Ponciano Garcia[3], Benítez Cardoza C[1]. beni1972uk@yahoo.com.mx, jlv64@hotmail.com.
[1]Laboratorio de Investigación Bioquímica, ENMyH, Instituto Politécnico Nacional; [2]LANGEBIO, CINVESTAV-Irapuato; [3]UAM-Cuajimalpa. México

Trichomonas vaginalis is a protozoan, the causal agent of trichomoniasis, the most common non-viral sexually transmitted infection (STI) spread worldwide. Trichomoniasis is associated with perinatal complications and infections in the genitourinary tract in both sexes. For over 40 years, the treatment against trichomoniasis is the provision of nitroimidazoles, commonly metronidazole and tinidazole. However, 5 to 20% of the patients show no improvement by this treatment. This highlights the need for new therapeutic regimens against trichomoniasis. Carbohydrates are the main nutrient source for *T. vaginalis*. Therefore, the enzymes in the glycolytic pathway on *T. vaginalis* like triose phosphate isomerase (TIM) are potential therapeutic targets. We performed molecular interaction simulations (*Docking*) between a set of compounds obtained from libraries and triose phosphate isomerase from *T. vaginalis*. Subsequently, the compounds with higher probability of interaction were assayed in their ability to inhibit or destabilize the mentioned glycolytic enzyme. Some compounds selected by docking strategies were able to reduce the replication and viability of *T. vaginalis* cultures. These findings have important implications in the development of new therapeutic strategies against trichomoniasis.

*In silico R*ational Enzyme Engineering of Manganese Peroxidase through Biophysical and Biochemical Modeling

Sandra Acebes[a], Elena Fernandez-Fueyo[b,c], Angel Martinez[b], Victor Guallar [a,d]

[a] *Barcelona Supercomputing Center (BSC). Joint BSC-CRG-IRB Research Program in Computational Biology, Barcelona, Spain*

[b] *Centro de Investigaciones Biológicas, CSIC, Madrid, Spain*

[c] *Delft University of Technology, Dept. of Biotechnology. Delft, The Netherlands*

[d] *Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain*

Nowadays, industrial processes demand more efficient, economical and environmental friendly processes, and in this route, enzymes pose a suitable solution. Since natural enzymes usually do not present the optimal properties that industry requires, it is sometimes convenient to tune them by protein engineering. In this regards, the application of computational techniques in the field of enzyme engineering supposes a great revolution, being especially powerful when combines with experimental data.

In this work, we joined dynamic ligand simulations with quantum mechanics calculations to provide a complete computational description of the enzymatic process where (i) biophysical simulations reproduce ligand diffusion and (ii) biochemical modeling samples the chemical event.

Ligand diffusion or dynamic motion can be studied typically by Molecular Dynamics (MD) simulation. However, ligand migration from the solvent to the binding site is sometimes far from MD time scales using standard computational power. For this reason, we studied the ligand binding phenomena using PELE [1], an algorithm that combines a Monte Carlo based algorithm with a protein structure prediction one, allowing to reproduce long time processes in only a few hours of CPUs. Then, the chemical reaction, which requires an explicit electron treatment, was described by methods based on Quantum Mechanics-Molecular Mechanics (QM/MM) calculations. In particular, we computed the electronic coupling [2] to estimate the oxidation probability.

Using such a broad analysis, we engineered a highly stable manganese peroxidase with putative industrial applications, activating the enzyme for new substrate oxidation after rational mutation of two nonconserved superficial residues[3]. Notably, we also predicted the change in the oxidation rate by computing the electronic coupling, achieving comparable experimental kinetic data.

In conclusion, from a complete computational description of the biophysical and biochemical events, we rational engineered an enzyme, which enhancement was confirmed by *in vitro* production and characterization. Overall, the capability of conducting such detailed studies and their match with experimental evidence underlines the importance of computational modeling in future enzymatic biotechnology.

References

1.- Borrelli, K.W., *et al.*, *PELE: protein energy landscape exploration. A novel Monte Carlo based technique.* Journal of Chemical Theory and Computation, 2005. 1(6): p. 1304-1311

2.- Acebes, S. Cabeza de Vaca, I., *et al.* eCoupling Server: A tool to compute and analyze electronic couplings. Journal of computational chemistry, 2016

3.- Acebes, S., *et al.*, *Rational Enzyme Engineering Through Biophysical and Biochemical Modeling.* ACS Catalysis, 2016. 6(3): p. 1624-1629

POLYMER NANOCOMPOSITE WITH GRAFTED NANOPARTICLES: STUDY OF ITS REOLOGY AND EQUILIBRIUM SPATIAL ORGANIZATION.

Carrasquedo Peñaloza Carlos Arturo[1,2], Manero Octavio[2], Castillo-Tejas Jorge[3], Aguayo Vallejo Juan Pablo[4].
[1]Facultad de Química, Universidad Nacional Autónoma de México. [2]Instituto de Investigaciones en Materiales, 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 Autónoma de Tlaxcala.

ABSTRACT

In this work, we applied equilibrium and nonequilibrium molecular dynamics simulation to obtain the spatial organization and material functions, respectively, of a model of polymer nanocomposite. The biggest challenge of polymer nanocomposite is improving nanoparticle dispersion; in this sense one of the approach is graft nanoparticle surface with chain chemically similar to matrix polymer, for this reason, there is a competition between tether-induced steric stabilization which can induce microphase ordering, and matrix-induced depletion-like attraction which can drive macrophase separation[1], and the spatial organization depends on the last factors. This equilibrium organization of nanoparticles directly disturbs the response of material to flow and in consequence the rheology of melt.

Our model system is based on literature, and meant to mimic a polymer nanocomposite composed of grafted spherical nanoparticles dissolved in a homopolymer melt where the matrix and grafted polymer are the same chemistry. We compare the actual results with the last research, where the dispersion of nanoparticles was made by simple shear flow varying intensity of energy attraction-repulsion impose by superficial area changing.

[1] A. Jayaraman and K. Schweizer, *Macromolecules* **41**, 9430(2008).

THE NON-DOMINANCE OF COUNTERIONS IN THE SIZE-SYMMETRIC AND VALENCE-ASYMMETRIC ELECTRIC DOUBLE LAYER

Enrique González-Tovar,[a] Guillermo Iván Guerrero-García,[b] Manuel Quesada-Pérez,[c] and Alberto Martín-Molina[d]

[a] Instituto de Física, Universidad Autónoma de San Luis Potosí, Mexico

[b] CONACYT–Instituto de Física, Universidad Autónoma de San Luis Potosí, Mexico

[c] Departamento de Física, Universidad de Jaén, Escuela Politécnica Superior de Linares, Spain

[d] Grupo de Física de Fluidos y Biocoloides, Departamento de Física Aplicada, Facultad de Ciencias, Universidad de Granada, Spain

ABSTRACT

In electric double layer (EDL) systems there is a proverbial fact known as *the dominance of the counterions* (DC). According to this mean-field prescription, the structural and thermodynamic properties of electrolyte solutions containing highly charged colloids or surfaces are determined by the characteristics of ions with an opposite polarity (or *counterions*). It is important to note that the DC phenomenon was originally established by assuming a *point-ions* model of the supporting electrolyte (i.e., on the basis of the Poisson-Boltzmann equation). Contrastingly, in a recent pair of papers, some of the present authors have showed that the inclusion of *ion correlations and finite ionic-size* effects in the EDL treatment implies, in fact, *the non-dominance of the counterions*. These previous studies were performed for EDLs with *size-asymmetric* and *valence-symmetric* ions. Here, we now report a complementary integral equation and Monte Carlo inquiry which evidences that the DC rule is also invalid in the reverse situation, namely for systems with *size-symmetric* and *valence-asymmetric* species. Therefore, our results prove that the non-dominance of counterions in the EDL is, by no means, an exclusive consequence of the size-asymmetry of an electrolyte next to charged interfaces.

Molecular confinement model with pressure and temperature effects.

Antonio Alvarez de la Paz (1), Ruben Santamaria (1), Tania González-García (1).

(1) Department of Theoretical Physics, Institute of Physics, UNAM, A.P.20-364, México Cd. Méx., México.

The aim of this work was to construct a molecular model from first principles with the capability of simulate pressure and temperature, in which the variables depend solely on the properties of the system. The above in order to perform a direct interpretation of the quantities involved with those that would be in a laboratory experiment. In addition, the model is able to perform measurements both at the microscopic level and at the macroscopic level. The model mimics the behavior of a pressure cooker, using a container with atomic structure as the pot, a thermal bath as the flame and the atoms of study like the soup. The dynamics governing equations of motion are derived from a Lagrangian function [1]. The effects of the thermal bath are obtained following the development of Zwanzig [2]. The interaction forces are calculated using ab-initio methods. The pressure effects are mechanically introduced by reducing the volume of the container. The Miller experiment [3] was chosen as an application of the model, obtaining relevant thermodynamic information such as an equation of state (E, V, T). Furthermore the method can be used to analyze other experiments under realistic conditions, for example: Clusters [4], DNA contaminants and even protein folding [5].

References

[1] Ruben Santamaria, Antonio Alvarez de la Paz, Luke Roskop, and Ludwik Adamowicz. Statistical contact model for confined molecules. *Journal of Statistical Physics*, 164(4):1000–1025, 2016.

[2] Robert Zwanzig. Nonlinear generalized langevin equations. *Journal of Statistical Physics*, 9(3):215–220, 1973.

[3] Stanley L. Miller. A production of amino acids under possible primitive earth conditions. *Science*, 117:528–529, 1953.

[4] Jacques Soullard, Ruben Santamaria, and Denis Boyer. Thermodynamic states of nanoclusters at low pressure and low temperature: The case of 13 h2. *The Journal of Physical Chemistry A*, 115(35):9790–9800, 2011. PMID: 21800887.

[5] Ruben Santamaria, Keith Jones, Maricela Arroyo, and Tania González-García. Polymer folding via external potentials in ab-initio calculations. *Computational and Theoretical Chemistry*, 1068:72 – 80, 2015.

Functional characterization of a putative hybrid diguanylate cyclase/phosphodiesterase protein from *Azospirillum brasilense* Sp245

Elvia G. Gómez Vázquez[1]; Antonio de J. Salazar Garcia[1]; Cesar Millán Pacheco[2]; Beatriz E. Baca[1]; Alberto Ramírez Mata[1].
1.- Centro de Investigaciones en Ciencias Microbiológicas, Benemérita Universidad Autónoma de Puebla. Av. San Claudio S/N Apartado Postal 72000, Puebla, Pue. aramirezmata@gmail.com.
2.- Facultad de Farmacia, Universidad Autónoma del Estado de Morelos. Av. Universidad No.1001, Chamilpa, Apartado postal 62209, Cuernavaca, Mor., México.

Azospirillum brasilense is one of the most selected Plant Growth-Promoting Rhizobacteria (PGPR) group. The bacterium promotes the growth and development of economically important crops, using several mechanisms such as phytohormone production, nitrogen fixation, phosphate solubilization, siderophores production. (1)
Effective colonization of plant roots by *Azospirillum* plays an important role in growth promotion. It is now common knowledge that bacteria in natural environments persist by forming biofilms. (2) Biofilms are highly structured, surface-attached communities of cells encased in a self-produced extracellular matrix, which protects bacteria from stress conditions and enhances bacteria-plant association. (3)
Cyclic diguanylate monophosphate (c-di-GMP) is a second messenger that regulates a variety of phenotypes, including biofilm formation, motility and virulence in multiple bacteria. The molecule is synthetized from two molecules of GTP by diguanylate cyclases (DGC) containing a GG(D/E)EF domain; while its degradation is accomplished by phosphodiesterases (PDE) with two different EAL or HD-GYP domains. (4)
The *A. brasilense* Sp245 genome encodes several GGDEF and EAL domain proteins (20 and 5, respectively), with asignificant fraction (~10) predicted to be multidomain (e.g.,GGDEF-EAL) enzymes containing an additional Per-Arnt Sim(PAS) sensor domain (5). However, the biochemical activities and physiological functions of these multidomain enzymes remain largely unknown.
Here, we present bioinformatic and biochemical analyses of a predicted PAS-GGDEF-EAL domain containing protein, AZOBR_40216, here named DGC/PDE-A. To this purpose we used the I-Tasser, VMD and Chimera programs. We used crystal structure of MorA from *Pseudomonas aeruginosa* (4RNF) (6). B) in the second way we expressed, purified and determined the PDE and DGC activity of the recombinant protein expressed in *E. coli* BL21 with the plasmid pGEX4T-1, to measure the activities we used as substrates, bis-(p-nitrophenyl) phosphate (Bis-4pNPP) and [α-^{32}P]-GTP, respectively.
Preliminary data about diguanylate cyclase and phosphodiesterase activities, the DGC/PDE-A has phosphodiesterase activity, because this enzyme breaks down the phosphodiester bond from Bis-4pNPP. On the other hand No diguanylate cyclase activity was observed.

1.- Bashan Y and de-Bashan L. 2010. How the plant growth promoting bacterium Azospirillum promotes plant growth – a critical assessment. In Advances in Agronomy, Vol. 108 (Sparks D, ed), pp. 77–136. Academic Press, Burlington.

2.- Guerrero-Molina, María F; Winik, Beatriz C; Pedraza, Raúl O. 2012 More than rhizosphere colonization of strawberry plants by Azospirillum brasilense. Applied Soil Ecology 61 205– 212.

3.- Costerton JW, Lewandowski Z, Caldwell DE, Korber DR, Lappin-Scott HM. Microbial biofilms. Annu Rev Microbiol. 1995. 49: 711-745.

4.- Römling U, Galperin M, Gomelsky M. (2013) Cyclic di-GMP: the first 25 years of a universal bacterial second messenger. Microbiol. Mol. Biol. Rev. 77.

5.- Wisniewski-Dyé F, Borziak K, Khalsa-Moyers G, Alexandre G, Sukkharnikov L, Wuichet K, *et al* (2011) *Azospirillum* genomes reveal transition of bacteria from aquatic to terrestrial environments. PLoS Gen. 7 (12).

6.- Phippen C.W., Mikolajek H., Schlaefli H.G., Keevil C.W., Webb J.S., Tews I. 2014. Formation and dimerization of the phosphodiesterase active site of the Pseudomonas aeruginosa MorA, a bi-functional c-di-GMP regulator. FEBS.p.588:4631-463.

Acknowledgements

Elvia Guadalupe Gómez Vázquez and Antonio de Jesús Salazar García, master students in Ciencias Microbiológicas (BUAP), is a recipient of master scholarships from the Consejo Nacional de Ciencia y Tecnología.

Study of Molecular Interactions between Carbon Nanotubes and Polyethylene Terephthalate (PET)

A. Rico-Campos, Edgar O. Castrejón-González*
Departamento de Ingeniería Química, Instituto Tecnológico de Celaya

Since the discovery of carbon nanotubes (CNTs) by Ijima in 1991, the CNT have aroused a great research interest due to its unique properties such as high electric and thermal conductivity, an excellent bending stiffness and tensile strength [1]. The CNTs form stable aggregates due to Van de Waals interactions, and these aggregates are so hard to disperse in polymer matrix [2]. In this work we performed Molecular Dynamics (MD) simulations to study π-π interactions between CNTs and polyethylene terephtalate (PET).

The π-π interactions are originated when two aromatic rings are positioned each other. These interactions are important non-covalent intermolecular forces, similar to hydrogen bonds. In the arrangement of aromatic rings one can generally distinguishes between an Stacked arrangement (face-face) and an edge (point-to-face) T-shaped conformation. Stacking has not necessarily to be a perfect face-to-face alignment of the atoms, but can also be an offset or slipped packing [3].

The analysis was performed in single wall CNT armchair type (10,10) pristine and functionalized with carboxyl, hydroxyl, amino and phenyl group respectively. The funcional groups were randomly placed with a proportion of 5\%. The PET chain was built with 10 monomers. The COMPASS force field was used to perform the MD simulation in an NVT ensemble at 300 K.

Results are depicted in the following table, where the best interaction is between functionalized CNT with hydroxil group and PET.

It can be observed that there is a trend in almost all systems (except NTC-OH), if there are more interactions π-π, the absolute value of the interaction energy is higher.

CNT type	**Interaction energy (kcal/mol)**	**Standard deviation**	**Average π-π interactions**	**Average radius of gyration**
Pristine	-93.8925	7.0366	7.7554	10.5770
NTC-COOH	-83.4197	8.049	2.75	7.7481
NTC-NH_2	-90.2378	7.7669	3.9882	7.6962
NTC-OH	-97.0676	6.7526	3.4167	9.7845

References

[1] D. Aztatzi-Pluma, Edgar O. Castrejón-González, *Study of the Molecular Interactions between Functionalized Carbon Nanotubes and Chitosan*, J. Phys. Chem. C 2016, 120, 2371-2378.

[2] O. Osazuwa,M. Kontopoulou, P. Xiang, Z. Ye, A. Docoslis, *Polymer composites containing non-covalently functionalized carbon nanotubes: A study of their dispersion characteristics and response to AC electric fields*, Procedia Eng. 2012, 42, 1414-1424.

[3] Christoph Janiak, *A critical account on _−_ stacking in metal complexes with aromatic nitrogen-containing ligands*, J. Chem. Soc., Dalton Trans., 2000, 3885-3896.

The interaction of sodium sulfite with the DNA nucleic acid bases: a first-principles molecular dynamics study

Daniel Martínez Zapata (1), Hortencia Rosas Acevedo (2), Rubén Santamaría (1).

(1) Department of Theoretical Physics Institute of Physics, UNAM, A.P. 20-364, Ciudad de México, México.

(2) FES-Zaragoza, UNAM, Ciudad de México, México.

The impact of contaminants on humans is a topic of general interest as they affect the human physiology. The sodium sulfite (Na_2SO_3) is an important derivative from SO_2 pollutant [1]. Recent investigations on these compounds have shown damages in rat hepatocytes [2], alterations of DNA, and cell apoptosis [3]. On the other hand, the nucleic acids DNA and RNA are the central molecules in the storage and processing of the genetic information of living forms [4]. In this respect, it is of paramount importance to investigate their behavior in the presence of contaminants. We are specifically interested on dealing with the DNA nucleic acid bases (*NAB*s) A, G, C, T and their interaction with Na_2SO_3, since, in principle, it is reactive to the *NAB*s and capable to produce malfunctioning of DNA with serious consequences on the genetic processes [5]. We use molecular dynamics to investigate the interaction of Na_2SO_3 with the DNA *NAB*s making use of the Born-Oppenheimer molecular dynamics method in combination with density functional theory [6, 7] to elucidate the different chemical reaction channels between Na_2SO_3 and the *NAB*s. The results on energetics, atomic charges, and electrostatic potentials provide evidence of relevant structural and chemical changes of the *NAB*s after interacting with Na_2SO_3 [8]. Therefore, sodium sulfite is concluded to have a destructive character on the *NAB*s.

References

[1] Z. Meng, G. Qin, B. Zhang, J. Bai, Mutagenesis. 19, 465-468, **2004**.

[2] H. Niknahad, P. J. O'Brien, Chem. Biol. Interact. 174, 147-154, **2008**.

[3] N. Sang, L. Hou, Y. Yun, G. Li, Ecotoxicol. Environ. Saf. 72 879-884, **2009**.

[4] James D. Watson, Tania A. Baker, Stephen P. Bell, Alexander Gann, Michael Levine, Benjamin Cummings, seventh ed. San Francisco, ISBN-13: 978-0321905376, **2014**.

[5] N. Uren, S. Yuksel, Y. Onal, Toxicol. Ind. Health. 30, 311-315, **2014**.

[6] A. D. Becke, Phys. Rev. A 38, 3098-3100, **1988**.

[7] C. Lee, W. Yang, R. G. Parr, Phys. Rev. B 37, 785-789, **1988**.

[8] R. Santamaria, G. Cocho, L. Corona, E. González, Chem. Phys. 227, 317-329, **1998**.

Study of the effect of THF on CH4 sII gas hydrates using MC simulations

Florianne Castillo-Borja[1], Richart Vázquez-Román[2], Ulises Iván Bravo Sánchez[1]
[1] Instituto Tecnológico de Aguascalientes, Departamento de Ingeniería Química
[2] Instituto Tecnológico de Celaya, Departamento de Ingeniería Química

Gas hydrates are nonstoichiometric crystalline inclusion compounds that consist of cages of different sizes and geometries where guest molecules such as N_2, CH_4 and CO_2 are trapped. These cages exist due to hydrogen bonds between water molecules. Guest molecules are encaged inside the cages giving stability to the hydrate [1]. Hydrates are formed at different conditions depending on the guest molecule but usually at temperatures near to 273 K and pressures of at least a few hundred of MPa. The need to require high pressures to maintain stability is the main drawback to give a practical and safe manner to the use of hydrates in different industrial processes. For this reason, hydrate formation promoters have been used to produce hydrates under less severe temperature and pressure conditions than those needed without the promoter. Some of these promoters include water soluble organic compounds such as tetrahydrofuran (THF). The presence of these promoters causes the formation of a binary hydrate where large cages are occupied by the promoter and small cages are occupied by the gas. CH_4 is known to forms simple hydrates with a cubic structure I (sI) and fill small and large cages. The stabilization of CH_4 simple sI hydrate requires higher pressure and lower temperature conditions in comparison with binary THF+CH_4 sII hydrate [2]. The hydrate formation pressure in the CH_4+THF+H_2O system at a given temperature reaches a minimum when THF concentration is around 5.6 % mol [2, 3]. However, increasing concentrations of promoter decreases this effect of pressure reduction and even concentrations above 10 mol % tend to thermodynamically inhibit the hydrate formation [4]. The existence of a critical concentration of CH_4 in binary THF+CH_4 hydrates has been detected by means of NMR measurements [5]. When hydrate is obtained from solutions where the mole ratio of THF was 5.6% at T = 268 K and P = 2 MPa, only CH_4 occupies the small cavities of binary hydrate; when the concentration of THF is diminished, it was observed that the occupation of large cavities for CH_4 can be possible. The amount of CH_4 in large cavities increases until reaching a maximum at a concentration of 0.2 mol % of THF under this critical concentration, CH_4 molecules occupy no more large cavities of the hydrate, disappearing completely from these cavities below THF concentration of 0.05 mol % [5]. By adjusting the concentration of THF in the liquid phase, it could be adjusted or tuned the amount of CH_4 molecules in the cavities of the binary hydrate.

In this work Monte Carlo simulations were performed on the Gibbs ensemble to study the effect of THF on the cage occupancies of binary THF+CH_4 sII hydrate. All the simulations were performed using the MCCCS Towhee software package [6]. The results achieved include the total occupancies for 293 K, 299 K and 303 K, the composition of the three phases in equilibrium, liquid, hydrate and vapor. It is observed that the use of the additive THF increases the amount of methane that can be stored in the large cavities of the sII hydrate, as it is the case for other gases that form binary THF hydrates. The angular order parameter showed that methane can be found within large cavities of sII hydrate at all the conditions analyzed. To analyze the effect of the concentration of the THF were performed simulations with different concentrations of THF in the liquid phase. It is shown that there is a concentration around the 3 % mol of THF in the liquid phase, which gets the largest occupation of methane in hydrate sII cages.

[1] Sloan E.D., Koh C.A. Clathrate hydrates of natural gases, 3rd edition, CRC Press, Boca Ratón, FL, 2007.
[2] Deugd R.M., Jager M.D., Arons J.S. Mixed hydrates of methane and water-soluble hydrocarbons modeling of empirical results. AIChE J. 2001, **47**, 693-704.
[3] Zhang Q., Chen G-J., Huang Q., Sun C-Y., Guo X-G, Ma Q-L. Hydrate formation conditions of a hydrogen+methane gas mixture in tetrahydrofuran+water. J. Chem. Eng. Data 2005, **50**, 234-236.
[4] Strobel T.A., Koh C.A., Sloan E.D. Thermodynamic predictions of various tetrahydrofuran and hydrogen clathrate hydrates. Fluid Phase Eq. 2009, **280**, 61-67.
[5] Kim D-Y., Park J., Lee J-W., Ripmeester J.A., Lee H. Critical guest concentration and complete tuning pattern appearing in the binary clathrate hydrates. J. Am. Chem. Soc. 2006, **128**, 15360-15361.
[6] MCCCS Towhee version 7.0.1, http://towhee.sourceforge.net

A study of the isotropic-nematic phase change in a dipole colloid due to an external field.

[1]C. Medel-Hernández, [2]M. González-Melchor, [1]R. Ramírez-Sánchez
[1]Facultad de ciencias Físico Matemáticas, BUAP
[2]Instituto de Física, BUAP

We study the ordering properties for a dipole colloidal system under the influence of an external field. The structure and ordering properties are calculated in terms of the order parameters. The order parameter are obtained through the orientational probability density function, given as the solution to the Smoluchowski equation in equilibrium, on the diffusive time scale.

We present results for the Isotropic-Nemática phase transition (I-N) and for the pre-transition of the dipole colloid. We analyze the curves of the probability density function (pdf), the autofactor of orientational structure and the orientational autodiffusion. Due to the symmetry of the dipole an axial nematic phase was expected, which was obtained from our results.

In order to show the congruence of the theoretical results with numerical results, we propose the use of Brownian Dynamics to analyze the translational and rotational motion of the particles. The rotation motion is expected to be influenced by the external field and the particles tend to be directed towards the latter.

[1]Medel-Hernández, C. (2016). Cambio de fase Isotrópico-Nemático inducido por un campo externo en un coloide dipolar, (Tesis de licenciatura) FCFM, BUAP. Puebla, México.

[2]Allen M. P & Tildesley D.J, (2006), Computer Simulation of Liquids, Great Britain, Oxford University Press.

[3]Satoh A, (2011) Introduction to Practice of Molecular Simulation, Akita Prefectural University Japan, Elservier.

[4]Ramírez-Sánchez, R. (2012). Propiedades orientacionales en cristales coloidales multipolares. (Tesis doctoral). FCFM, BUAP. Puebla, México.

[5]Ramírez-Sánchez, R., Ruíz-Estrada, H. (2012). Orientational distribution for dipolar and quadrupolar colloids driven by an external field. Revista Mexicana de Física, 58, 104.

Molecular dynamics simulation of pcb interacting with 2,4-dichloro biphenyl for environmental proposal

Ana Karen Estrada-Rodríguez[1,2], Carlos A. García-Pérez[1*], Aldo Vega Esquivel[1], Ángel D. Reyes-Figueroa[3], Sofía Alvarado-Reyna[2].
[1]Centro de Biotecnología Genómica, Instituto Politécnico Nacional, [2]Universidad Autónoma de Tamaulipas, [3]Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional.
*** Corresponding author**: Carlos A. García-Pérez, carlosgarcía@usal.es

The Persistent Organic Pollutants (POPs) have multiple toxic properties, they are resistant to degradation, bioaccumulate and transported by air, water and even by migratory animals [1]. The a Polychlorinbated Biphenyls Compounds (PCBs), have the highest impact on the environment, and are considered a xenobiotic compound that causes damage to the environment and to humans [2][3]. Thus, it represents an opportunity for investigation. The aim of the present work is to analyze, through different bioinformatic tools, the interaction of the compound biphenyl bichlorate (2,4-dichloro biphenyl) with the protein 2,3-dihidroxybiphenyl dioxygenase (pdb: 1kw9). The crystal structure has the compound 2,3-dihidroxybiphenyl, which was used to measure its affinity to the protein in order to define a threshold. Molecular dynamics is one of the most widely used methods to analyze the movement of particles between atoms and molecules over a period of time. This technique will allow us to simulate the interaction of the compound with the protein, to observe behavior and stability of the compound at the binding site. From the molecular docking, the pose between the protein and the ligand with higher affinity was obtained. The compound 2,4-dichloro biphenyl interacts with amino acids HIS208, PHE201, VAL147 and TYR249. Moreover, the 2,3-dihidroxy biphenyl compound also interacts with these amino acids. It is worth mentioning that in both cases the score, when performing docking with AutoDock [4], was -6.5. From the molecular dynamics, the following results were obtained, in the RMSD analysis of C-alpha in time, from ns 60, it showed a stabilization of the complex, similar to that reached in the ns 50 of protein without the compound. The fluctuations occurring at the binding site of the compound in the complex. It shows higher similarity with the protein. The molecular docking results showed that the compounds interact with the same amino acids and obtain the same affinity. This suggests that there is a high possibility that the protein can be used as a 2,4-dichloro biphenyl carrier. On the other hand, analyses performed with molecular dynamics make clear that the behavior of this protein will be similar to the behavior of the complex.

References

[1] R. Boopathy, “Bioremediation: Principles and practices, volume I. Fundamentals and applications. Subhas K. Sikdar and Robert L. Irvine, Technomic Publishing Company, Inc., Lancaster, PA, (1998), 765 pages, [ISBN No.: 1-56676-308-8], U.S. List Price: $164.95,” *Environ. Prog.*, vol. 18, no. 4, pp. W5–W6, 1999.

[2] R. W. Macdonald, L. A. Barrie, T. F. Bidleman, M. L. Diamond, D. J. Gregor, R. G. Semkin, W. M. J. Strachan, Y. F. Li, F. Wania, M. Alaee, L. B. Alexeeva, S. M. Backus, R. Bailey, J. M. Bewers, C. Gobeil, C. J. Halsall, T. Harner, J. T. Hoff, L. M. M. Jantunen, W. L. Lockhart, D. Mackay, D. C. G. Muir, J. Pudykiewicz, K. J. Reimer, J. N. Smith, G. . Stern,

W. H. Schroeder, R. Wagemann, and M. B. Yunker, “Contaminants in the Canadian Arctic: 5 years of progress in understanding sources, occurrence and pathways,” *Sci. Total Environ.*, vol. 254, no. 2, pp. 93–234, 2000.

[3] S. N. Pentyala, M. Rebecchi, S. Mishra, A. Rahman, R. Stefan, J. Rebecchi, and P. R. S. Kodavanti, “Polychlorinated Biphenyls : In situ Bioremediation from the Environment OF,” pp. 249–262, 2011.

[4] G. M. Morris, R. Huey, W. Lindstrom, M. F. Sanner, R. K. Belew, D. S. Goodsell, and A. J. Olson, “AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility,” *J. Comput. Chem.*, vol. 30, no. 16, pp. 2785–2791, 2009.

Modeling of human cystatin C – chymopapain dimer and molecular dynamics simulations

David Octavio Tovar Anaya, Ponciano García Gutiérrez and Rafael A. Zubillaga.

Departamento de Química, Área de Biofisicoquímica, Universidad Autónoma Metropolitana Unidad Iztapalapa, San Rafael Atlixco 186, Col. Vicentina, 09340 Ciudad de México. 58044674. david_tvquim@hotmail.com.

The human cystatin C – chymopapain dimer was initially modeled by docking the human cystatin C X-ray structure (PDB code 3GAX) to the crystallographic structure of chymopapain (PDB code 1YAL) using the pyDockWeb server. We used the restricted versión of pyDock (RST), which imposes constraints on the posible interface contacts. The atomic model of the homologus papain – stefin B complex (PDB code 1STF) and the amino acid sequence alignments between chymopapain and papain, and human cystatin C and stefin B indicated the possible interface residues. The model with the lowest RMSD respect to the crystallographic structure of papain - stefin B complex was selected as the starting structure for further refinement by molecular dynamics simulations.

Molecular dynamics (MD) simulations were performed using GROMACS 5.0 software with the OPLS force field. The side-chain ionization states in the separate proteins and in the complex at the various pH values were established using the pKa values estimated using PROPKA. The human cystatin C - chymopapain model was placed in the center of a periodic cubic box, with 10 Å between the complex and the edge of the box. A total of 30800 SPC/E water molecules were needed to fill the box, and 13 chloride ions were needed to neutralize the net protein charge. MD simulation was performed using an NPT ensemble at 300 K and 1.0 bar for 350 ns. A LINCS algorithm was applied to constrain the length of all covalent bonds, and a 2 fs time step was used.

The resulting RMSD reached an equilibrium which tells us that the human cystatin C – chymopapain complex is stable.

Inserción de una superficie FCC de platino en un fullereno por medio de Dinámica Molecular DFT

Karen de la Mora Zarco, Juan Horacio Pacheco Sánchez
División de Estudios de Posgrado e Investigación del Instituto Tecnológico de Toluca
Av. Tecnológico s/n. Col. Agrícola Bellavista, Metepec 52149, Estado de México
e-mail: jpachecos@toluca.tecnm.mx

Using DFT an fcc surface of four platinum atoms was geometrically optimized, then the resulting surface was set to interact with a C_{60} fullerene molecule trough a DFT molecular dynamics (Using DMol^3 BIOVIA Materials Studio) in order to insert the platinum surface in a fullerene molecule. The fullerene deformation is a transition to amorphous carbon only in the half surface attacked by the platinum surface. We are looking for a surface of activated carbon by platinum as catalyzer support of an electrode un a fuel cell. DFT m-GGA/M06-L calculations are all electron, unrestricted spin polarization, dnd basis, fermi orbital occupation, C1 symmetry group. Molecular dynamics calculations are NVE ensemble, T=300 K, Time step 1 fs, 50 steps, 0.05 of total simulation time, max Memoru 2048 MB, charge 0.

Usando DFT se optimizó geométricamente una superficie fcc de cuatro átomos de platino, y se puso en interacción con una molécula de fullereno C_{60}. Después se usó dinámica molecular DFT DMol^3 de BIOVIA Materials Studio para insertar la superficie de platino en el fullereno. Se observa la deformación del fullereno a carbón amorfo en solo la mitad afectada por el platino. Los cálculos realizados para DFT m-GGA/M06-L son all electron, unrestricted spin polarization, dnd basis, fermi orbital occupation, C_1 symmetry group. Los cálculos de dinámica molecular son NVE ensemble, T=300K, Time step 1 fs, 50 steps, 0.05 of total simulation time, Max. Memory = 2048 MB, charge 0. Se busca una superficie de carbon activada por platino como soporte del catalizador en un electrodo de una celda de combustible.

Short time self orientational diffusion coefficient for a multipolar colloids.

Erwin Ramírez Solano, erwin.31@hotmail.com , Facultad de Ciencias Físico Matemáticas, BUAP.

Minerva González Melchor, minerva@ifuap.buap.mx, Instituto de Física, BUAP.

Roberto Ramírez Sánchez, rramirez@fcfm.buap.mx, Facultad de Ciencias Físico Matemáticas, BUAP.

Behavior of the short time self orientational diffusion coefficient in the induced isotropic-nematic phase is investigated with the Smoluchowski equation, because the crystallization is a process driven by local motions, short time diffusion. [1, 3]

The suspension used is composed by hard spherical particles with an incrustation punctual multipole in their centers of mass with low structured and driven by external homogeneous field. We report results for dipole and quadrupole moments using numerical analysis for distinct values of the external field.

The diffusion in this suspensions depend on the degree of order in the state of the system and the electric external field.

In our model, the diffusion coefficient is described by order parameters, Legendre [2].

Implementing Brownian dynamics, we investigate the behavior of the short time self orientational diffusion coefficient for the multipolar colloids [4].

[1] P. G. de Gennes and J. Prost, The Physics of liquid crystals, second edition (Clarendon Press-Oxford, 1998).

[2] O. Alarcón-Waess and E. Diaz-Herrera, Phys. Rev.E 65, 031402 (2002).

[3] R. Ramírez Sánchez, Propiedades orientacionales en cristales coloidales multipolares, Phd thesis, BUAP, 2012.

[4] M. González. IFUAP-BUAP, Brownian dynamics.

Electrolyte-Mediated Assembly of Charged Nanoparticles

Sumit Kewalramani[1], Guillermo I. Guerrero-García[1,2], Liane M. Moreau[1], Jos W. Zwanikken[1], Chad A. Mirkin[1,3], Monica Olvera de la Cruz[1,3,4], and Michael J. Bedzyk[1,3,4]
[1] Materials Science and Engineering Department, Northwestern University, Evanston, Illinois 60208, United States
[2] Instituto de Física, Universidad Autónoma de San Luis Potosí, Àlvaro Obregón 64, 78000 San Luis Potosí, San Luis Potosí, Mexico
[3] Department of Chemistry, Northwestern University, Evanston, Illinois 60208, United States
[4] Physics and Astronomy Department, Northwestern University, Evanston, Illinois 60208, United States

Solutions at high salt concentrations are used to crystallize or segregate charged colloids, including proteins and polyelectrolytes via a complex mechanism referred to as "salting-out". Here, we combine small-angle X-ray scattering (SAXS), molecular dynamics (MD) simulations, and liquid-state theory to show that salting-out is a long-range interaction, which is controlled by electrolyte concentration and colloid charge density. As a model system, we analyze Au nanoparticles coated with noncomplementary DNA designed to prevent interparticle assembly via Watson–Crick hybridization. SAXS shows that these highly charged nanoparticles undergo "gas" to face-centered cubic (FCC) to "glass-like" transitions with increasing NaCl or $CaCl_2$concentration. MD simulations reveal that the crystallization is concomitant with interparticle interactions changing from purely repulsive to a "long-range potential well" condition. Liquid-state theory explains this attraction as a sum of cohesive and depletion forces that originate from the interelectrolyte ion and electrolyte–ion–nanoparticle positional correlations. Our work provides fundamental insights *into the effect of ionic correlations* in the salting-out mechanism and suggests new routes for the crystallization of colloids and proteins using concentrated salts.

ACS Cent. Sci., 2016, 2 (4), pp 219–224
DOI: 10.1021/acscentsci.6b00023

MODELING OF THE PROCESS OF OXYGEN ABSORPTION AND DESORPTION AT THE MITOCHONDRIAL LEVEL

[1]JOSÊ JUAN PEÑA LEAL, [2]ARTUTO LUNA, [3] MARIA FERNANDA CERVANTES PÊREZ, [4]BART. GUZMÂN GUEVARA

[1] ICN, CCC, UNAM, [2]F.CIENCIAS, UNAM, [3]IEMS CUAJIMALPA, [4] IIM, UNAM,

ABSTRAC

The ability to absorb or reject oxygen at the mitochondrial level is a very important process in the functioning of biological organisms. The mitochondria is a multifunctional organism, and for the proper functioning of this, the absorption or elimination of oxygen is vital. We present the advances obtained in the modeling of this important process, using the stochastic matrix model, which we have been using to model oxidation processes and reduction of thin films of cerium.

Molecular dynamic simulation of the interaction Pb2+ and the enzyme Glutathione S-transferaza

Susana Lozano Muñiz (2)., F. Noé Mendoza Ambrosio (1).

(1) Instituto de Química Aplicada, (2) Instituto de Biotecnologı́a, Universidad del Papaloapan,
Circuito Central #200, colonia Parque Industrial, Tuxtepec, Oax., México C.P. 68301.

We studied two molecular interaction, the fist one among Pb2+[1] and the ligand Glutathione GSH and the second interaction among Pb2+ and the enzyme Glutathione-S-transferases GST with the molecular dynamic methodology[2]. The objective in this research was trial the pair potential for Pb2+ with small peptides and proteins that was obtained from literature. First, we analyzed the interaction in water (SPC/E) for reproduce the coordination number and structural similarity. Second, we build a molecular simulation GSH, Pb2+ with NaCl in water for reproduce the coordination number[3] and the more frecuently interactions in the peptide[4]. Finally, we localize the Pb2+ in the most probable site into the protein GST and made some nanoseconds of MD for check the stability in the site and obtain some properties in function of time.

References

[1] K. J. Johnson, R. T. Cygan, J.B. Fein, *Geochimica et Cosmochimica Acta* , 70, 5057, **(2006)**

[2] Frenkel, D. and Smit, B., *Understanding Molecular Simulation: From Algorithms to Applications*, Computational science series, Elsevier Science, **2001**.

[3] Araujo A. S., Sonoda M. T., Piro O. E., Castellano E. E., *J. Phys. Chem. B*, 111, 2219-2224, **2007**.

[4] Kirberger M., J. J. Yang, *J. Inorg. Biochem.*, 102, 1901-1909. **2008**.

Numerical evidence of quasicrystals from a simple model in two dimensions

Perez-Lemus Gustavo R.[a], Ramirez-Hernandez Abelardo[c], Armas-Perez Julio C.[a,b]* and Quintana H. Jacqueline[a]*
[a] Instituto de Química, Universidad Nacional Autónoma de México, 04510 D.F., Mexico
[b] División de Ciencias e Ingenierías, Campus León, Universidad de Guanajuato, Loma del Bosque 103, León (Gto.) 37150, Mexico
[c] Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, USA

*Corresponding Authors email: jc.armas@ugto.mx, jaq@correo.unam.mx

Abstract

Monte Carlo simulations have been performed to study the phase behavior of a binary mixture of soft corona systems. Each species has a hard core disk decorated by a soft corona that is repulsive for equal species and attractive for different component. Each component hold a different corona radius. A wide variety of structures is generated by changing the corona radius as well as the proportion of the species.

Exploring the Phase Behavior of Diblock Copolymers using Discontinous Molecular Dynamics

Susana Marín-A.[1], Jacqueline Quintana-H.[1], Gustavo A. Chapela[2], Adrián Martínez-G.[3]
[1]Instituto de Química, Universidad Nacional Autónoma de México; 04510, Cd. Méx.
[2] Departamento de Físico, Universidad Autónoma Metropolitana-Iztapalapa, 09340, Cd. Méx.
[3]Institute of Molecular Engineering, University of Chicago, 60637, Illinois, USA
e-mail: susyma3005@gmail.com

Copolymers are a type of polymer formed by two or more different kinds of monomers joined by covalent bonds. Copolymers present microphase separation due to the nature of the intermolecular interactions between the different species, this have mulltiple aplications, such as production of complex microchips, medical aplications and synthesis of materials with enhanced properties, increasing interest for studying this kind of materials. These systems have been wide studied both theoretically and experimentaly.

This study was focused in modelling the phase behavior of dyblock copolymers using Discontinuous Molecular Dynamics, in order to get a better landscape on diblock copolymers phase diagrams. We used a simple model of linear chains which interact by means of square wells. Different computations were acquired and compared changing the length (5, 6, 7, 8 and 10 monomers), composition, flexibility and temperature.

We found some of the characteristic phases in copolymers (lamelar and cylindric phases), for their characterization we calculate the density profiles, order parameter and radial distribution function.

Gaucher G., Dufrense M. H. Sant V. P., et. al. Block copolymer micelles: preparation, characterization and application in drug delivery, Journal of Controlled Release **2005**, 1091 169-188
Matesen M. W. Effect of Architecure on the Phase Behavior of AB-Type Block Copolymer Melts, Macromolecules **2012**, 45, 2161-2165
Chapela G. A., Martínez-Casas S. E. and Alejandre J., Molec. Phys. **1984,** 53, 139

MODELING OF THE PROCESS OF OXYGEN ABSORPTION AND REJECTION AT THE MITOCHONDRIAL LEVEL

[1]José Juan Peña Leal, [2]Arturo López Luna, [3]María Fernanda Cervantes Pérez, [3]Daniela Nava Hernández [4]Bart. Guzmán Guevara

[1] Instituto de Ciencias Nucleares, Laboratorio de Átomos Fríos, Dpto. Física de Plasmas y Radiaciones, U.N.A.M., A.P. 70-543, 01000 –Ciudad de México, México, UNAM, [2]Facultad de Ciencias, UNAM, Ciudad de México, México, UNAM, [3]IEMS CUAJIMALPA, Ciudad de México, México, [4] IIM, Ciudad Universitaria, UNAM, Ciudad de México, México

SUMARY

The ability to absorb or reject oxygen at the mitochondrial level is a very important process in the functioning of biological organisms. The mitochondria is a multifunctional organism, and for the proper functioning of this, the absorption or elimination of oxygen is vital. We present the advances obtained in the modeling of this important process, using the stochastic matrix model, which we have been using to model oxidation processes and reduction of thin films of cerium.

TOPOLOGICAL DEFECTS IN TWO-DIMENSIONAL LIQUID CRYSTALS

ITZEL I. JULIO BORJA(1), JULIO C. ARMAS PÉREZ(2), JACQUELINE QUINTANA HINOJOSA (1)

(1) *Instituto de Química, Universidad Nacional Autónoma de México, México 04510 D.F., México.*

(2) *División de Ciencias e Ingenierías, Campus León, Universidad de Guanajuato, Loma del Bosque 103, León (Gto.) 37150, México.*

We have performed numerical simulations to study topological deformations: kind *splay and bend*, that arose from imposition of homeotropic anchoring in two-dimensional liquid crystals [1]. Our molecular model is the bent hard needles whith repulsive interactions only [2]. Metropolis Monte Carlo simulations in the canonical ensemble was used [3]. Previous results showed the existence of defects for this molecular model for bulk systems [4]. Our results shows that homeotropic anchoring plays a definite role in the kind of defects. We notice that the deformations depend of parameters molecular. We compute the free energy Frank to determinate the kind of defect.

References

[1] E. B. Priestley, Peter J. Wojtowicz, and Ping Sheng. Introduction to liquid crystals. Plenum Press, **1979**.

[2] J. Peón, J. Saucedo-Zugazagoitia, F. Pucheta-Mendez, R. Perusquía, G. Sutmann and J. Quintana-H. *The Journal of Chemical Physics 125, 104908*, **2006**.

[3] M. P. Allen and D. J. Tildesley, Computer Simulation of liquids. Clarendon Press, Oxford, **1990**.

[4] R. Perusquía, J. Peón and J. Quintana-H. Physica A 345, 130-142, **2005.**

Effects of adsorption of Ag, Au, Pt and Pd clusters on the conductivity of graphene.

R. M. Del Castillo (1,2), L. E. Sansores (2)
(1) Instituto Mexicano del Petróleo, Eje Central Lázaro Cárdenas Norte 152, Ciudad de México, C.P. 07730.
(2) Instituto de Investigaciones en Materiales, UNAM, 04510, México

We present adsorbate effects of metallic cluster on single-layer graphene. We performed a DFT study of the adsorption of silver, gold, platinum and palladium cluster with n atoms (n=1, 2, 3 and 4). Also, we analyzed the electronic structure and the conductivity of this systems. The conductivity was accomplished according to a model formulate by Katsnelson et al. [1], where the adsorption sites are the scattering centers of our systems. The scattering mechanisms is likely to be controlled by ripples (microscopic corrugation of a graphene sheet) and for those it is creates a long-range scattering potential, Coulomb scatterers. The conductivity can be easily measured as a result that the charge-carrier mobility and it is independent of carrier concentration, in agreement with experimental observation [2, 3]. We find that in some cases (Ag) a fixed number of atoms impurities, the formation of clusters enhances the mobility and improve the electrical conductivity.

References

[1] M. I Katsnelson, A. K. Geim, Phil. Trans. R. Soc. A, **366,** 195-204 (2008)

[2] K. S. Novoselov et al. Nature **438**, 197-200 (2005)

[3] Y. Zhang, Y. Tan, H. L. Stormer, P. Kim, Nature, **438**, 201-204 (2005)

Stability of cocrystals by Molecular Dynamics simulations

Frank José Salas, Edgar Núñez-Rojas and José Alejandre
Universidad Autónoma Metropolitana – Unidad Iztapalapa

A cocrystal is a system with at least two components that can be solids or liquids at room conditions. Molecules in a cocrystal interact by hydrogen bonds producing a new crystal which has different properties than the original compounds.

In the present work it was studied by molecular dynamics simulations the formic acid/pyridine and the isonicotinamide/formamide cocrystals at 173 K and 150 K, respectively. The OPLS/AA force field is used with two set of parameters for the liquids: a) the original set obtained by matching the simulations results to experimental density and heat of vaporization at room conditions and b) new values that reproduce the dielectric constant, surface tension and density at different temperatures. The parameters of pyridine and formamide have been published previously (Salas FJ et al.(2015) J. Chem. Theory Comput. 11(2):683). The liquid formic acid is parameterized in this work using the same procedure. The new parameters improved the predictions of the original values. The isonicotinamide parameters are obtained from those of pyridine and formamide assuming they are transferable. The structure and stability of cocrystals are determined through the calculation of distances and angles of atoms that form hydrogen bonds in different molecules. The simulation results were compared with experimental measurements of X-ray diffraction and a good agreement is found.

Parameterization of acetone and its application in aqueous solutions.

Edith N. De Jesús González (1,2), Alexander Pérez de la Luz(2), José Alejandre
Ramírez(2), Jorge López Lemus(1).

(1) Facultad de Ciencias, Universidad Autónoma del Estado de México. Instituto Literario No. 100, Col. Centro, 50000, Toluca Estado de México.

(2) Departamento de Química. Universidad Autónoma Metropolitana-Iztapalapa. Av. San Rafael Atlixco No. 186, Col. Vicentina, Iztapalapa, 09340, Ciudad de México, México.

We applied a systematic procedure [1] to improve the OPLS/AA intermolecular parameters of acetone [2] using molecular dynamics simulations[3]. In this work, the atomic charges were calculated using a new approach applied directly to the total molecular electronic density[4] with a continuous solvent model[5] to include polarizability effects around an isolated molecule. The charges and short ranged interaction parameters were scaled linearly to reproduce the experimental dielectric constant, liquid-vapor surface tension and liquid density at room conditions. The self-difussion coefficient and heat of vaporization were also calculated. The new set of parameters were used to simulate, with the TIP4P/ε water model[6], aqueous solutions at different acetone concentrations. All the calculated properties of pure and binary mixtures are in excellent agreement with experimental data and they improved those from the OPLS/AA force field.

[1] F. J. Salas, G. A. Méndez-Maldonado, E. Núñez-Rojas, G. E. Aguilar-Pineda, H. Domíngez, J. Alejandre, *J. Chem. Comput.* 11, 683-693, **2015.**

[2] W. L. Jorgensen, D. S. Maxwell, J. T. Rives, *J. Am. Chem. Soc.* 118, 11225, **1996.**

[3] M. P. Allen and D. J. Tildesley, *Computer Simulation of liquids.* Clarendon Press, Oxford, **1990.**

[4] F. L. Hirshfeld, *Theoret. Chim. Acta.* 44, 129-138, **1977.**

[5] A. V. Marenich, C. J. Cramer, D. G Truhlar, *J. Phys. Chem. B.* 113, 6378-6396, **2009.**

[6] R. Fuentes-Azcatl, J. Alejandre, *J. Phys. Chem. B.* 118, 1263-1272, **2014**.

Development of all atom force fields based on the total molecular electronic density

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

Having good force fields of polar liquids is fundamental to understand, from molecular point of view, several phenomena in a wide range of scientific and technological applications in chemistry, physics, biology and engineering. In recent works we have shown that force fields such as OPLS/AA[2], GAFF[3] and CHARMM[4] fail to reproduce the solubility of liquids with different degree of polarization[formamida]. The problem is related with the value of the molecular dipole moment, obtained from electronic structure calculation of isolated molecules, which is not able to reproduce the experimental dielectric constant in the liquid phase and the surface tension at the liquid-vapor interface. We will present in this work a new route to assign the charge distribution of atoms in molecules based in the total molecular density [Hirshfeld]. Several polar liquids, pure components and binary mixtures, with dielectric constant going from 15 to 180 are studied using a systematic procedure to obtain the interaction parameters [Salas] of a new all atoms force field. The simulation results for dielectric constant, surface tension, liquid density, heat of vaporization and self-diffusion coefficient at room conditions have excellent agreement with experimental data, which shows the power of the method.

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.

Assessment of MOF's structure quality: quantifying defects content in crystalline porous materials.

Nadeen Al-Janabi, Xiaolei Fan, and Flor R. Siperstein
School of Chemical Engineering and Analytical Science University of Manchester

Metal Organic Frameworks (MOFs) have attracted the interest of many researchers due to their potential applications in separations, however understanding the actual properties of the materials are hindered by inconsistencies in reported experimentally measured isotherms, such as those reported for CO_2 adsorption on $Cu_3(BTC)_2$. $Cu_3(BTC)_2$ is a well-known open-metal site MOF that is constructed by coordinatively linking unsaturated copper sites with benzene tricarboxylate (BTC) ligands rendering a microporous structure with tetrahedron-shaped side pockets (~5Å opening), square-shaped principal pores (~11Å and ~13.5Å) and triangular windows (~3.5Å). We used Grand Canonical Monte Carlo (GCMC) simulations to investigate the effect of different structural defects (some reactants and solvent molecules) in MOFs principal pores and side pockets in addition to copper vacancies on CO_2 adsorption on $Cu_3(BTC)_2$. Molecular simulations were used to generate collections of hypothetical and well characterized MOF samples' adsorption isotherms, that were later used to assess the quality of experimentally prepared materials in-house and others reported in the literature. Specific and accessible surface area of all the defective MOF models were also calculated and showed that the materials with the same surface area can have different adsorption capacities depending on the nature of structural defects. Using the collection of the simulated adsorption isotherms, a metric was developed to assess the structural quality of real materials, in which, the amount adsorbed measured experimentally is the weighted sum of all the calculated adsorption isotherms of the defective structures.

Reference:

[1] Al-Janabi N, Fan X, Siperstein FR. J Phys Chem Lett. 2016, 21;7(8):1490-4. doi:10.1021/acs.jpclett.6b00297.

What is the molecular phenotype of amyloid fibrils derived from amyloid-beta peptide variants involved in Alzheimer's Disease?

Carlos Z. Gómez-Castro and Alberto Vela

Departamento de Química del Centro de Investigación y Estudios Avanzados del Instituto Politécnico Nacional. Av.
Instituto Politécnico Nacional 2508 Col. San Pedro Zacatenco, 07360 México, D.F. México.
email: carloszepgc@gmail.com

Amyloid fibrils are one of the main hallmarks of the Alzheimer's Disease (AD) eventough the precise role of these protein aggregates in neurodegeneration is not fully understood. There are many variants of the amyloid-beta (Aβ) peptide, main component of amyloid fibrils, that have been associated to disease-modifying phenotypes. For instance, the Tottori variant replaces the Asp7 residue for an Asn in the peptide sequence and is responsible for increasing amyloid fibril formation and producing a familiar type of AD.[1-3] In the case of rodent Aβ, the substitutions R5G, Y10F, and H13R produce a reduced capability to form amyloid fibrils and to develop AD-related pathology. This variant was also reported to be less prone to form β-sheet structure and to have less capacity to accumulate transition metals.[4,5]

Thus, in this work we evaluated these observations in molecular models of amyloid fibrils bearing this amino acid substitutions and comparing structural features to the human wild-type sequence. Molecular dynamics simulation of these models showed that the strucutre of the N-terminal domain is very sensitive to these amino acid substitutions and that several features of the amyloid fibrils such as the secondary structure incidence would be affected. These molecular features may be directly connected to the known phenotype observed in these naturally-occuring variants.

References

1. Wakutani, Y.; Watanabe, K.; Adachi, Y.; Wada-Isoe, K.; Urakami, K.; Ninomiya, H.; Saido, T. C.; Hashimoto, T.; Iwatsubo, T.; Nakashima, K., Novel amyloid precursor protein gene missense mutation (D678N) in probable familial Alzheimer's disease. *J. Neurol. Neurosurg. Psychiatry* **2004**, *75* (7), 1039- 1042.
2. Hori, Y.; Hashimoto, T.; Wakutani, Y.; Urakami, K.; Nakashima, K.; Condron, M. M.; Tsubuki, S.; Saido, T. C.; Teplow, D. B.; Iwatsubo, T., The Tottori (D7N) and English (H6R) familial Alzheimer disease mutations accelerate A beta fibril formation without increasing protofibril formation. *J. Biol. Chem.* **2007**, *282* (7), 4916-4923.
3. Ono, K.; Condron, M. M.; Teplow, D. B., Effects of the English (H6R) and Tottori (D7N) Familial Alzheimer Disease Mutations on Amyloid beta-Protein Assembly and Toxicity. *J. Biol. Chem.* **2010**, *285* (30), 23184-23195.
4. Johnstone , E. M.; Chaney, M. O.; Norris, F. H.; Pascual, R., Little, S.P., Conservation of the sequence of the Alzheimer's disease amyloid peptide in dog, polar bear and five other mammals by cross-species polymerase chain reaction analysis. *Mol. Brain Res.* **1991**, *10* (4), 299-305.
5. Leskovjan, A. C.; Lanzirotti, A.; Miller, L. M., Amyloid plaques in PSAPP mice bind less metal than plaques in human Alzheimer's disease. *Neuroimage* **2009**, *47* (4), 1215-1220.

Reparametrization of force fields for nitrogen compounds in liquid phase

Jorge A. Aguilar-Pineda and José Alejandre
Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, México Distrito Federal, México

In previous works, it has been shown that the obtaining of new parameters of force fields for highly polar systems following the systematic methodology of Salas et al. we reproduce thermodynamic properties that are in good agreement with experimental data in both, pure components and mixtures. In this work, we present the reparametrization of the force field of four molecules belonging to the family of nitroalkanes: nitromethane, nitroethane, 1-nitropropane and 2-nitropropane, in addition to urea. In the case of nitroalkanes, the study was carried out by taking the atomic charges obtained by the population analysis of Mulliken at a theory level M062x / 6-311 ++ g ** with solvent effect. The scaling of the parameters in both, atomic charges and Lennard-Jones, was performed in two ways: taking the individual parameters of each atom and using the concept of transferability, identifying the atoms CNH_2 as a transferable group. In the case of urea, the parameters obtained in the reparametrization of acetamide united atom were taken as the base, replacing the methyl group with the group NH_2 of the same molecule. At 298.15K the urea is presented in solid state so the study was performed in a mixture with water at different urea concentrations. The target thermodynamic properties in both, pure compounds and in mixtures, were dielectric constant, surface tension and liquid density. In all cases, the results are in good agreement with the experimental data.

Suitable Binding Mode of Niflumic acid to Ca^{2+}-activated Cl^{-} channel studied by Combined Molecular Docking/Dynamics methods

García-Pérez Carlos Armando (1), Aguirre Alvarado Charmina (2), Rodríguez Páez Lorena (2), Cordero Martínez Joaquín (3), Enrique Othón Hernández-González (3).

[1]Centro de Biotecnología Genómica, Instituto Politécnico Nacional, Reynosa Tamaulipas, México
[2]Escuela Nacional de Ciencias Biológicas, Instituto Politécnico Nacional Ciudad de México.
[3]Departamento de Biología Celular, Centro de Investigación y Estudios Avanzados del Instituto Politécnico Nacional, Ciudad de México.

INTRODUCTION.

CaCCs are anionic channels related to transepithelial ion transport, smooth muscle contraction, olfaction, phototransduction, nociception and control of neuronal excitability [1]. Recently, the proteins TMEM16A and B were identified as CaCCs found in all eukaryotes [2]. Pharmacological blockers are useful for testing the physiological role of CaCCs channels in various cells and tissues. Niflumic acid (NFA) is a reversible inhibitor of CaCCs [3]. The molecular mechanism through this blocker produce its effect on CACCs is practically unknown. In the present study we used the X-ray extracellular domain of TMEM16 (4WIS; PDB) from fungus *Nectria haematococca* to performed docking and molecular dynamic simulations to find suitable TMEM16-NFA molecular interactions. The molecular docking performed with AutoDock 4.2.6 showed that after 100 poses performed with 5 000 000 evaluations, the pose between the protein and NFA with higher affinity (ΔG= -3.9 cal/mol) interacts with M355, F362, F358 I527, A531, L547, K543 and I551. The dynamic behavior of NFA-TMEM16 A complex was evaluated by 60 ns using Gromacs 5.0.5. The Root-mean-square deviation (RMSD) analysis of C-alpha in time, from ns 40, it showed a stabilization of the complex. Nevertheless, at present time the simulation it is running until reach the 100 ns, and it is notice that could be stabilized at 100 ns. The RMS fluctuations occurring at the binding site of the compound in the complex, showing a high fluctuation between atoms 3000 to 7000.

REFERENCES.

1. Pedemonte N, Galietta LJ. 2014. Structure and function of TMEM16 proteins (anoctamins). Physiol Rev 94(2):419-59.

2. Liu Y, *et.al.*. 2015. Characterization of the effects of Cl^{-} channel modulators on TMEM16A and bestrophin-1 Ca^{2+} activated Cl^{-} channels. Pflugers Arch 467(7):1417-1430.

3. Bradley E, *et.al.* 2014. Pharmacological characterization of TMEM16A currents. Channels (Austin) 8(4):308-2.

Computer coarse-grained model of Bax protein interacting with a lipid bilayer

Ana Fernanda Salazar Maldonado, Jorge Luis Rosas Trigueros, Rosaura Palma Orozco
Laboratorio Transdisciplinario de Investigación en Sistemas Evolutivos, Escuela Superior de Cómputo, Instituto Politécnico Nacional; Ciudad de México, México

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 of at least 25 members. The first identified homologue of this nature was Bax. During the apoptotic process, Bax migrates from the cytosol to the mitochondria due to a conformational change in the protein. Subsequently, Bax forms oligomers which form pores on the outer membrane. This way, at least another 5 pro-apoptotic agents are released, that contribute to the degradation of the celular structures in different ways. This events are required in order for the apoptotic process to continue. Recent studies show the importance of lipids in the apoptosis regulation. This work proposes a coarse grained model of the interaction between Bax and a lipid bilayer that could contribute to understand the role both elements play in the apoptotic process.

Computational coarse-grained models of the proteins HERG1 and HERG1B.

Rosaura Palma Orozco, Jorge Luis Rosas Trigueros
Laboratorio Transdisciplinario de Investigación en Sistemas Evolutivos
LaTrISE-SEPI-ESCOM, Instituto Politécnico Nacional, México
rpalma@ipn.mx

Tumor cell lines have been found which preferentially overexpress the HERG1 gene and a truncated N-terminal form (HERG1B), forming heterotetramers. Blocking these channels prevents growth of such tumor cells. In silico studies of proteins and their mutants may reveal important information about their structure and function. Previous studies reveal the enormous computational complexity involved in atomistic simulations of the channel inserted into the membrane. In order to perform simulations of the membrane/protein system, a coarse grained (CG) modeling is proposed in this work. This methodology will allow to study the evolution of the system in relevant time scales. The models to be obtained from CG-HERG1 and CG-HERG1B will be of great help, since they will obtain simplified models of the protein reducing the original number of atoms but conserving its essential properties. This study aims to provide insight into their role in the proliferation of tumor cells. This can help in understanding apoptosis and conditions such as cancer.