

# INFORME DE ACTIVIDADES DEL 2006

## 1. Publicaciones

### Investigación

- J Garza, R Vargas, A Cedillo, M Galván and PK Chattaraj
- Comparison between the frozen core and finite differences approximations for the generalized spin-dependent global and local reactivity descriptors in small molecules
- *Theor. Chem. Acc.* **115** [4] 257-265 (2006)
  
- A Cedillo
- Density functional theory models of reactivity based on an energetic criterion
- En *Theoretical Aspects of Chemical Reactivity*, A. Toro-Labbé (Ed.)
- ISBN 0-444-52719-2, pp 27-35, Elsevier (2006)
  
- Á Vazquez-Mayagoitia, R Vargas, JA Nichols, P Fuentealba and J Garza
- Relationship between singlet-triplet excitation energies and the Kohn-Sham orbitals obtained with potentials that exhibit a wrong asymptotic behaviour
- *Chem. Phys. Lett.* **419**, 207-212 (2006)
  
- N Aquino, J Garza, A Flores-Riveros, JF Rivas-Silva and KD Sen
- Confined helium atom low-lying s-states analyzed through correlated Hylleraas wave functions and the Kohn-Sham Mode
- *J. Chem. Phys.* **124**, 054311 (2006)
  
- MH Matus, J Garza and M Galván
- The effect of double bonds on the conducting properties of ciguatoxin 3C and tetrahydropyrane based polymers: A theoretical study
- *J. Phys. Chem. B.* **110**, 1172-1178 (2006)
  
- JL Gázquez, A Cedillo, B Gómez and A Vela
- Molecular fragments in density functional theory
- *J. Phys. Chem. A* **110** [13] 4535-4537 (2006)
  
- JZ Ramírez, R Vargas, J Garza y BP Hay
- Performance of the Effective Core Potentials of Ca, Hg, and Pb in Complexes with Ligands Containing N and O Donor Atoms
- *J. Chem. Theory and Comput.* **2**, 1510-1519, (2006)
  
- C Frontana, A Vazquez-Mayagoitia, J Garza, R Vargas, I Gonzalez
- Substituent Effect on a Family of Quinones in Aprotic Solvents: An Experimental and Theoretical Approach
- *J. Phys. Chem. A.* **110**, 9411-9419 (2006).
  
- J Ireta, J Neugebauer, M Scheffler, A Rojo y M Galván
- Structural Transitions in the Polyalanine  $\alpha$ -Helix under Uniaxial Strain
- *J. Am. Chem. Soc.* **127**, 17241-17244 (2005)
  
- M Gothelid, H von Schenck, J Weissendrieder, B Akerman, A Tkatchenko, M Galvan.
- Adsorption site. Core level shifts and charge transfer on the Pd(111)-I( $\sqrt{3}\times\sqrt{3}$ )surface.
- *Surf. Sci.* **600**(15) 3093-3098 (2006).

- A Tkatchenko, N Batina, M Galvan
- Potential energy landscape of monolayer surface system governed by repulsive lateral interactions: the case of (3x3)-I-Pt(111).
- *Phys. Rev. Lett.* **97**(3) 036102 (2006).
- B Gómez, NV Likhanova, MA Domínguez-Aguilar, R Martínez-Palou, A Vela y JL Gázquez
- Quantum chemical study of the inhibitive properties of 2-pyridyl-azoles
- *J. Phys. Chem. B* **110**, 8928-8934 (2006).

### **Divulgación**

- M Galván y J Ireta
- Impacto y perspectivas del Estudio de la Estructura Electrónica de Proteínas.
- En “*La Física Biológica en México: Temas Selectos*”, Coordinadores, L García-Colin Scherer, L Dagdug, P Miramontes y A Rojo, El Colegio Nacional, México 2006, p.279-298.

### **2. Alumnos graduados**

- Tesis de Doctorado
- Posgrado en Química UAM-I
- Ma. De los Angeles Cuán Hernández
- Graduado
- Doctorado en Ciencias
- Posgrado en Química, UAM-I
- María de Lourdes Romero Villafranco
- Graduado

#### ***Otras asesorías académicas***

- Verano de la Investigación Científica del Pacífico
- Licenciatura QFB
- Mariano Méndez Chávez
- 100%

### **3. Profesores visitantes e invitados**

- Felipe Aparicio Platas
- UAM-Cuajimalpa
- Estructura electrónica de biomoléculas
- 2006-2007

### **4. Eventos organizados**

- V Reunión Mexicana de Físicoquímica Teórica
- San Luis Potosí, SLP
- 16 a 19 de Noviembre de 2006.
- Miembro del Comité Organizador.