

INFORME DE ACTIVIDADES DEL 2005

1. Artículos

Publicados

- A. Cuan, J. M. Martínez Magadan, I. García-Cruz y M. Galvan
- Quantum Chemical Study of the HZSM-5-cyclohexene interaction pathways
- J. Mol. Catal. A **236**, 194-205, (2005)
- P.K. Chattaraj, N. Gonzalez-Rivas, M.H. Matus y M. Galvan
- Substituent Effects
- J. Phys. Chem. A **109**, 5602-5607 (2005)
- R. Meza, B. Gordillo y M. Galvan
- Local HSAB principle in the conjugate addition of p-substituted thiophenols to cyclohexenone
- Int. J. Quant. Chem. **104**, 29-37 (2005)
- A. Tkachenko, N. Batina, A. Cedillo y M. Galvan
- Charge Transfer and Adsorption energies in the iodine-Pt(111) interaction
- Surf. Sci. **581**, 58-65 (2005)
- A. Cuán, M. Galván y P. K. Chattaraj
- A philicity based análisis of adsorption of small molecules in zeolites
- J. Chem. Sci. **117**, 1-8 (2005)
- J. Garza, J. Z. Ramírez and R. Vargas
- The role of Hartree-Fock and Kohn-Sham orbitals in the basis set superposition error for systems linked by hydrogen bonds
- J. Phys. Chem. A. **109**, 643-651 (2005) *
- R. Vargas, J. Garza, R. A. Friesner, H. Stern, B. P. Hay, D. A. Dixon
- Reply to Comment on "Strength of the N-H...O=C and C-H...O=C Bonds in Formamide and N-Methylacetamide Dimers"
- J. Phys. Chem. A **109**, 6991-6992 (2005)
- J. Garza, R. Vargas, N. Aquino and K. D. Sen
- DFT reactivity indices in confined many-electron atoms
- J. Chem. Sciences. **117**, 379-386 (2005)
- R. Vargas, J. Garza and A. Cedillo
- A Koopmans-like approximation in the Kohn-Sham method and the impact of the frozen core approximation on the computation of the reactivity parameters of the density functional theory
- J. Phys. Chem. A **109**, 8880-8892 (2005)
- F. Méndez, M. L. Romero y J. L. Gázquez
- Chemical Reactivity of Hypervalent Silicon Compounds: The local hard and Soft Acids and Bases Principle
- J. Chem. Sci. **117**, 525-531 (2005)
- N. González-Rivas and A. Cedillo
- Performance of density functional theory methods to describe intramolecular hydrogen shifts
- J. Chem. Sci. **117**, 555-560 (2005)

Aceptados

- J. Garza, R. Vargas, A. Cedillo, M. Galván and P. K. 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.
- N. Aquino, Jorge Garza, A. Flores-Riveros, J. F. Rivas-Silva and K. D. Sen
- Confined helium atom low-lying s-states analyzed through correlated Hylleraas wave functions and the Kohn-Sham Model
- J. Chem. Phys.
- M. H. Matus, J. Garza and M. Galván
- The effect of double bonds on the conducting properties of ciguatoxin 3C and tetrahydropyran based polymers: A theoretical study
- J. Phys. Chem. B
- Á. Vazquez-Mayagoitia, R. Vargas, J. A. 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 behavior
- Chem. Phys. Lett.
- A. Cedillo
- Density functional theory models of reactivity based on an energetic criterion, en *Theoretical Aspects of Chemical Reactivity*, A. Toro-Labbé (Ed.)
- Elsevier

Memorias

- J. Radilla, M. Galván, Y. Trinidad-Reyes y N. Batina
- STM Image Simulation: Effect of the number of Tunneling States and the Isosurface Value
- Mater. Res. Soc. Symp. Proc. **838E**, 2005

Divulgación

- R. Vargas
- La fuerza del puente de hidrógeno débil y su papel en la estructura de los materiales
- Materiales Avanzados 2005, 5, 17-20, 2005

2. Alumnos graduados

- Proyecto terminal
- Licenciatura en Química, UAM-I
- Orlando Martínez Zapata
- Graduado
- Tesis de Maestría
- Posgrado en Química, UAM-I
- Nelly Ma. de la Paz González Rivas
- Graduado
- Tesis de Maestría
- Posgrado en Química UAM-I
- Hilda Macrina Santillán Vargas

- Graduado

3. EVENTOS ORGANIZADOS POR EL AREA

- 4ª Reunión Mexicana de Fisicoquímica Teórica
- Chihuahua, CHIU.
- Noviembre 2005