

# **Curriculum Vitae - Dr. Alvaro Posada-Amarillas**

## **PERSONAL DETAILS**

**NAME:** Alvaro Posada-Amarillas

**Date of Birth:** February 17th, 1960, **Birthplace:** Esperanza, Sonora, México,

**Nationality:** Mexican, **Sex:** Male, **Marital Status:** Married, **Children:** 3

**INSTITUTION:** Department of Research in Physics, Universidad de Sonora

**TITLE:** Full-time Researcher

**NATIONAL RESEARCHER:** S.N.I. 3

**TIMES CITED WITHOUT SELF-CITATION:** ~900 (h-index = 12)

**JOURNAL REFEREE:** J. Phys. Chem. C, Phys. Chem. Chem. Phys., Int. J. Quantum Chem., J. Non-Cryst. Solids, J. Nanoparticle Res.

**EDITORIAL BOARD MEMBER:** J. Appl. Surf. Interface

**ADDRESS:** Villa Rica #17, Fracc. Villa Sol, 83240 Hermosillo, Son.

### **CONTACT DETAILS:**

**Tel:** +52 662 2893792

**Cel:** +52 6622783643

**E-mail:** posada@cifus.uson.mx

## **UNIVERSITY EDUCATION**

Dr. PHYSICS OF MATERIALS    Centro de Investigación Científica y de Educación  
Jan 1992-Jul 1996                    Superior de Ensenada, Ensenada, B.C., México

M.Sc. PHYSICS                    Departamento de Investigación en Física, Universidad de Sonora,  
Aug 1985-Jul 1987                    Hermosillo, Sonora, México.

B.Sc. PHYSICS                    Departamento de Física, Universidad de Sonora, Hermosillo, Sonora,  
Jan 1980-Jun 1985                    México.

## EMPLOYMENT

### UNIVERSIDAD DE SONORA

- 1983** Research Assistant, Department of Physics
- 1985** Subject professor, Department of Mathematics
- 1985** Fixed-time Academic Technician, Department of Research in Physics
- 1987** Full-time Professor, Department of Physics
- 1988** Full-time Academic Technician, Department of Research in Physics
- 1997** Full-time Researcher, Department of Research in Physics

## RESEARCH GRANTS

"Computer simulation of binary metallic systems", National Council of Science and Technology (CONACYT), Project No. 35224-E, 2000-2003.

"Structure, stability and catalytic activity of Pd/Pt and Ni/Pd nanoparticles: Theoretical and experimental studies", National Council of Science and Technology (CONACYT), Project No. 24060, 2007-2012.

"Theoretical and experimental studies of supported bimetallic nanoparticles", National Council of Science and Technology (CONACYT), Project No. 180424, 2013-2017.

## NETWORKS

Member of COST Action MP0903: NANOALLOY - Nanoalloys as advanced materials: from structure to properties and applications.

### Research Visits

- 1999** Centro de Ciencias de la Materia Condensada, UNAM. Ensenada, B.C., México
- 2005** School of Chemistry, University of Birmingham, Birmingham, U.K.
- 2006** Max Planck Institute for Solid State Research, Stuttgart, Germany
- 2010** Max Planck Institute for Solid State Research, Stuttgart, Germany
- 2013** School of Chemistry, University of Birmingham, Birmingham, U.K.

### Research Interests

Computer simulation of liquid and amorphous metals; energetics and growth of metal clusters and nanoalloys; structural and electronic properties of clusters and crystals; synthesis

of metal clusters and nanoalloys and their catalytic activity; supported clusters; nanotechnology; local and global optimization algorithms.

## Scientific Publications

- “Vibrational properties of nickel and gold clusters”, S. Carnalla, A. Posada and I.L. Garzón, *Nanostructured Materials* **3**, pp. 385-390, 1993.
- “Microstructural analysis of simulated liquid and amorphous nickel”, Alvaro Posada-Amarillas and Ignacio L. Garzón, *Physical Review B* **53**, 8363(1996).
- “Vibrational analysis of Ni<sub>n</sub> clusters”, Alvaro Posada-Amarillas and Ignacio L. Garzón, *Physical Review B* **54**, 10362(1996).
- “Structural and vibrational analysis of amorphous Au<sub>55</sub> clusters”, Ignacio L. Garzón and Alvaro Posada-Amarillas, *Physical Review B* **54**, 11796(1996).
- “Lowest energy structures of gold nanoclusters”, I.L. Garzón, K. Michaelian, M.R. Beltrán, A. Posada Amarillas, P. Ordejón, E. Artacho, D. Sánchez Portal, and J.M. Soler, *Physical Review Letters* **81**, 1600(1998).
- “Structure and thermal stability of gold nanoclusters: The Au<sub>38</sub> case”, I.L. Garzón, K. Michaelian, M.R. Beltrán, A. Posada Amarillas, P. Ordejón, E. Artacho, D. Sánchez Portal, and J.M. Soler, *European Physical Journal D* **9**, 211(1999).
- “Electronic Properties and Chemical Bonding of Orthorhombic Chromium Carbide”, A. Posada-Amarillas, D.H. Galván, F.F. Castellón and M. Ávalos-Borja, *physica status solidi (b)* **229**, 1353 (2002).
- “Temperature effect on the local order of liquid Ni, Ag and Pb: A molecular dynamics study”, E. Urrutia-Bañuelos, A. Posada-Amarillas, I.L. Garzón, *Physical Review B* **66**, 144205(2002).
- "Extended Huckel tight-binding calculations of the electronic structure of YbFe<sub>4</sub>Sb<sub>12</sub>, UFe<sub>4</sub>P<sub>12</sub>, and ThFe<sub>4</sub>P<sub>12</sub>", Donald H. Galván, N. R. Dilley, M. B. Maple, A. Posada-Amarillas, Armando Reyes-Serrato, and J. C. Samaniego Reyna, *Physical Review B* **68**, 115110 (2003).
- “Structural and Dynamical Properties in Liquid Ni and Ag by Computer Simulation”, E. Urrutia-Bañuelos and A. Posada-Amarillas, *International Journal of Modern Physics B* **17** (7), 1011 (2003).
- “Experimental and theoretical DOS in Ni and Co silicides”, M. García-Méndez, M.H. Farías, D.H. Galván-Martínez, A. Posada-Amarillas, and G. Beamson, *Surface Science* **532-535**, 952 (2003).
- “Efecto de la Temperatura en las Propiedades Estructurales y Dinámicas de Ag líquida: Un Estudio con Dinámica Molecular”, E. Urrutia Bañuelos, A. Posada Amarillas, *Revista Mexicana de Física* **50**, 53 (2004).

- "Experimental and theoretical study of the electronic properties of CoSi<sub>2</sub> and NiSi<sub>2</sub>", M. García-Méndez, D. H. Galván, A. Posada-Amarillas, M. H. Farías, *Applied Surface Science* **230**, 386 (2004).
- "Electronic properties of Co and Ni silicides: a theoretical approach using extended Huckel method", D. H. Galván, A. Posada-Amarillas, J.C. Samaniego Reyna, M. García-Méndez, M. H. Farías, *physica status solidi (b)* **241**, 2905-2913, (2004).
- "Assessment of growth of silver nanoparticles synthesized from an ethylene glycol-silver nitrate-polyvinylpyrrolidone solution", A. Slistan-Grijalva, R. Herrera-Urbina, J. F. Rivas-Silva, M. Ávalos-Borja, F. F. Castellón-Barraza and A. Posada-Amarillas, *Physica E* **25**, 438-448, (2005).
- "Classical theoretical characterization of the surface plasmon absorption band for silver spherical nanoparticles suspended in water and ethylene glycol", A. Slistan-Grijalva, R. Herrera-Urbina, J. F. Rivas-Silva, M. Ávalos-Borja, F. F. Castellón-Barraza, A. Posada-Amarillas, *Physica E* **27**, 104-112 (2005).
- "Theoretical study of the electronic properties of PrM<sub>2</sub>B<sub>2</sub>C (M=Co,Ni,Pt)", Donald H. Galván, A. Durán, A. Posada-Amarillas, and R. Escudero, *Physical Review B* **74**, 245121 (2006).
- "Relationship between excess entropy and microstructure of undercooled liquid metals", Alvaro Posada-Amarillas, Efrain Urrutia-Bañuelos, Roberto Núñez-González, Dora J. Borbón-González, and Ignacio L. Garzón, *Journal of Non-Crystalline Solids* **353**, 2157 (2007).
- "Structures and energetics of 98-atoms Pd-Pt nanoalloys: Potential stability of the Leary tetrahedron for bimetallic nanoparticles", Lauro Oliver Paz-Borbón, Thomas V. Mortimer-Jones, Roy L. Johnston, Alvaro Posada-Amarillas, Giovanni Barcaro, and Alessandro Fortunelli, *Physical Chemistry Chemical Physics* **9**, 5202 (2007).
- "Synthesis of silver nanoparticles in a polyvinylpyrrolidone (PVP) paste, and their optical properties in a film and in ethylene glycol", A. Slistan-Grijalva, R. Herrera-Urbina, J.F. Rivas-Silva, M. Ávalos-Borja, F.F. Castellón-Barraza, A. Posada-Amarillas, *Materials Research Bulletin* **43**, 90 (2008).
- "Structure and stability of In<sub>X</sub><sup>Z</sup> (X≤9; Z=-1,0,1) clusters. Theoretical insights", A.F. Jalbout, A. Posada-Amarillas, A. Ordóñez-Campos, G. Moreno-Armenta, D.H. Galván. *Chemical Physics Letters* **464**, 58 (2008).
- "First principles calculations of the band gap of Al<sub>x</sub>Ga<sub>1-x</sub> and In<sub>x</sub>Ga<sub>1-x</sub>N", R. Núñez-González, A. Reyes-Serrato, A. Posada-Amarillas, D.H. Galván, *Revista Mexicana de Física* **54**, 111 (2008).
- "Diffraction patterns observed in two-layered graphene and their theoretical explanation", D.H. Galván, A. Posada-Amarillas, N. Elizondo, S. Mejía, E. Pérez-Tijerina, and M. José-Yacamán, *Fullerenes, Nanotubes and Carbon Nanostructures* **17**, 258 (2009).

- “Structural insights into 19-atom Pd/Pt nanoparticles: a computational perspective”, D.J. Borbón-González, R. Pacheco-Contreras, A. Posada-Amarillas, J.C. Schön, R.L. Johnston, and J.M. Montejano-Carrizales, *The Journal of Physical Chemistry C* **113**, 15904 (2009).
- “Metallic States at the Edges of MoS<sub>2</sub> Clusters”, D.H. Galván, A. Posada-Amarillas, and M. José-Yacamán, *Catalysis Letters* **132**, 323 (2009).
- “Energetic and structural analysis of 102-atom Pd-Pt nanoparticles: a composition-dependent study”, R. Pacheco-Contreras, A. Arteaga-Guerrero, D.J. Borbón-González, A. Posada-Amarillas, J.C. Schön and R.L. Johnston, *Journal of Computational and Theoretical Nanoscience* **7**, 199 (2010).
- “Effect of Proton Irradiation on Graphene Layers”, D. H. Galvan, A. Posada-Amarillas, S. Mejía, C. Wing, and M. José-Yacamán, *Fullerenes, Nanotubes and Carbon Nanostructures* **18**, 1 (2010).
- “A Theoretical Kohn-Sham DFT based study of Pt@Pd<sub>12</sub>”, Maribel Dessens-Félix, Rafael Pacheco-Contreras, Catalina Cruz-Vázquez, Alvaro Posada-Amarillas, Andreas M. Köster, *Journal of Computational and Theoretical Nanoscience* **7**, 1443-1446 (2010).
- “DFT calculation of the electronic properties and EEL spectrum of NiSi<sub>2</sub>”, Roberto Núñez-González, Armando Reyes-Serrato, Donald H. Galván, Alvaro Posada-Amarillas, *Computational Materials Science* **49**, 15-20 (2010).
- “Study of vacancies and Pd atom decoration on the electronic properties of bilayer graphene”, D.H. Galván, A. Posada-Amarillas, R. Núñez-González, M. José-Yacamán, S. Mejía, *Journal of Superconductivity and Novel Magnetism* **23**, 1543-1550 (2010).
- "Synthesis and Characterization of Copper Sulfide Nanoparticles Obtained by the Polyol Method", F. F. Castellón-Barraza, M. H. Farías, J. H. Coronado-López, M. A. Encinas-Romero, M. Pérez-Tello, R. Herrera-Urbina, and Alvaro Posada-Amarillas, *Advanced Science Letters* **4**, 596-601 (2011)
- "Concentration-dependent study of electronic and optical properties of c-Si and c-Si:H", R. Núñez-González, A. Posada-Amarillas, D. H. Galván, and A. Reyes-Serrato, *physica status solidi (b)* **248**, 1712–1717 (2011).
- "Experimental and theoretical properties of S–Mo–Co–S clusters", D.H. Galvan, Francis Leonard Deepak, Rodrigo Esparza, A. Posada-Amarillas, R. Núñez-González, X. Lopez-Lozano, M. Jose-Yacamán, *Applied Catalysis A: General* **397**, 46-53, (2011).
- “Tetrahelix Conformations and Transformation Pathways in Pt<sub>1</sub>Pd<sub>12</sub> Clusters”, Rafael Pacheco-Contreras, Maribel Dessens-Félix, Dora J. Borbón-González, L. Oliver Paz-Borbón, Roy L. Johnston, J. Christian Schön, and Alvaro Posada-Amarillas, *The Journal of Physical Chemistry A* **116**, 5235–5239 (2012).

- “Computational Study of Au<sub>4</sub> Cluster on a Carbon Nanotube with and without Defects using QM/MM Methodology”, Diana Barraza-Jiménez, D. H. Galvan, Alvaro Posada-Amarillas, Manuel Alberto Flores-Hidalgo, Daniel Glossman-Mitnik and Miguel José-Yacamán, *Journal of Molecular Modeling* **18**, 4885-4891 (2012).
- "Theoretical insights on the storage of carbon dioxide using single-walled carbon nanotubes", Chia M. Chang, Aned de Leon, Alvaro Posada-Amarillas, and Abraham F. Jalbout, *Computational Materials Science* **63**, 191–196 (2012).
- “Green-chemical synthesis of monodisperse Au, Pd and bimetallic (core-shell) Au-Pd, Pd-Au nanoparticles”, Eduardo A. Larios-Rodríguez, F.F. Castellón-Barraza, Ronaldo Herrera-Urbina, Dora J. Borbón-González, Alvaro Posada-Amarillas, *Advanced Science, Engineering and Medicine*, **5**, 665-672 (2013).
- "Theoretical study of amino acids encapsulation in zigzag single-walled carbon nanotubes", Chia M. Chang, Hsiao L. Tseng, Aned de León, Alvaro Posada-Amarillas, Abraham F. Jalbout, *Journal of Computational and Theoretical Nanoscience* **3**, 521-526 (2013).
- "Structures and electronic structure of neutral (CuS)<sub>N</sub> clusters (N=1-6): a DFT approach", Octavio J. Juárez-Sánchez, Nancy Perez-Peralta, Ronaldo Herrera-Urbina, Mario Sanchez, Alvaro Posada-Amarillas, *Chemical Physics Letters*, **570**, 132-135 (2013).
- "Determination of the energy landscape of Pd<sub>12</sub>Pt<sub>1</sub> using a combined Genetic Algorithm and Threshold Method", R. Pacheco-Contreras, Dora J. Borbón-González, M. Dessens-Félix, R. L. Johnston, J. C. Schön, M. Jansen, Alvaro Posada-Amarillas, *RSC Advances*, **3**, 11571–11579 (2013).
- "Structural Motifs of Bimetallic Pt<sub>101-x</sub>Au<sub>x</sub> Nanoclusters", Maribel Dessens-Félix, Rafael Pacheco-Contreras, Giovanni Barcaro, Luca Sementa, Alessandro Fortunelli, and Alvaro Posada-Amarillas, *The Journal of Physical Chemistry C* **117**, 20967–20974 (2013).
- "Exceptional oxidation activity with size-controlled supported gold clusters of low atomicity", Avelino Corma, Patricia Concepción, Mercedes Boronat, Maria J. Sabater, Javier Navas, Miguel José Yacaman, Eduardo Larios, Alvaro Posadas, M. Arturo López-Quintela, David Buceta, Ernest Mendoza, Gemma Guilera and Alvaro Mayoral, *Nature Chemistry* **5**, 775-781 (2013).
- "Experimental and Theoretical Properties of MoS<sub>2+x</sub> Nanoplatelets", D. H. Galvan, A. Posada-Amarillas, N. Elizondo, M. José-Yacamán, *Modern Research in Catalysis* **2**, 164-171 (2013).
- "Global Minimum Pt<sub>13</sub>M<sub>20</sub> (M = Ag, Au, Cu, Pd) Dodecahedral Core–Shell Clusters", Dora J. Borbón-González, Alessandro Fortunelli, Giovanni Barcaro, Luca Sementa, Roy L. Johnston, and Alvaro Posada-Amarillas, *The Journal of Physical Chemistry A* **117**, 14261-14266 (2013).

- "A theoretical study of Cu clusters in siliceous erionite", Joel Antúnez-García, D.H. Galván, A. Posada-Amarillas, Vitalii Petranovskii, *Journal of Molecular Structure* **1059**, 232-238 (2014).
- "Theoretical DFT study of homonuclear and binary transition-metal dimer", A. Posada-Borbón, A. Posada-Amarillas, *Chemical Physics Letters*, **618**, 66-71, 2015.
- "A DFT study of copper-oxide clusters embedded in dry and water-immersed siliceous mordenite", J. Antúnez-García, D.H. Galván, V. Petranovskii, A. Posada-Amarillas, *Computational Materials Science*, **106**, 140-148, 2015.
- "Electronic Properties of EuRu<sub>4</sub>P<sub>12</sub> Skutterudite", *Journal of Superconductivity and Novel Magnetism*, J. Antúnez-García, R. Núñez-González, D.H. Galván, A. Posada-Amarillas, **28**, 2171-2175, 2015.
- "Theoretical study of the thermally induced structural fluctuations in sub-nanometre size gold clusters", J. M. Cabrera-Trujillo, J. M. Montejano-Carrizales, F. Aguilera-Granja, A. Posada-Amarillas, *European Physical Journal D*, **69**, 167-175, 2015.
- "Assessment of Functionals for First-Principle Studies of the Structural and Electronic Properties of  $\delta$ -Bi<sub>2</sub>O<sub>3</sub>", D. H. Galván, R. Núñez-González, R. Rangel, P. Alemany, A. Posada-Amarillas, *Advances in Condensed Matter Physics*, DOI: 10.1155/2015/120294, 2015.
- "Exploring the energy landscape of Pt<sub>x</sub>Au<sub>115-x</sub> nanoalloys", Maribel Dessens-Félix, Rafael Pacheco-Contreras, J. M. Cabrera-Trujillo, J. M. Montejano-Carrizales, Lauro Oliver Paz-Borbón, Alessandro Fortunelli, Alvaro Posada-Amarillas, *Computational and Theoretical Chemistry*, **1074**, 150-156, 2015.
- "Computational Studies of Stable Hexanuclear Cu<sub>l</sub>Ag<sub>m</sub>Au<sub>n</sub> (l + m + n = 6; l, m, n > 0) Clusters", Alvaro Posada-Amarillas, Rafael Pacheco-Contreras, Sharity Morales-Meza, Mario Sanchez, and J. Christian Schön, *International Journal of Quantum Chemistry*, **116**, 1006-1015, 2016.
- "Experimental and theoretical analyses of ZnO nanoparticles deposited onto single-wall carbon nanotubes", D. H. Galvan, G. Alonso, M. Tejada, A. Torres, B. Reesja-Jayan, D. Ferrer, A. Posada-Amarillas, D. Barraza-Jimenez and M. José-Yacamán, *Fullerenes, Nanotubes and Carbon Nanostructures*, **24**, 541-546, 2016.
- "DFT study of composites formed by M<sub>2</sub> metallic clusters (M = Ni, Cu, Fe and Au) embedded in faujasite", Joel Antúnez-García, A. Posada-Amarillas, D. H. Galván, E. Smolentseva, V. Petranovskii and Sergio Fuentes Moyado, *RSC Advances*, **6**, 79160-79165, 2016.
- "Combined DFT and NBO Approach to Analyze Reactivity and Stability of (CuS)<sub>n</sub> (n=1-12) Clusters", J. Octavio Juárez-Sánchez, Donald H. Galván, Alvaro Posada-Amarillas, *Computational and Theoretical Chemistry*, **1103**, 71-82, 2017.
- "Synthesis of Au<sub>core</sub>Pd<sub>shell</sub> Nanoparticles by a Green Chemistry Method and Characterization by HAADF-STEM Imaging", Eduardo A. Larios-Rodríguez, F. F.

Castillón-Barraza, Ronaldo Herrera-Urbina, Ulises Santiago, Alvaro Posada-Amarillas, *Journal of Cluster Science*, DOI: 10.1007/s10876-017-1200-6, 2017.

## Book Chapters

*Chapter 10*, Moiré Patterns Observed in Bi Layer Graphene, Irradiated with High Energetic Protons, D. H. Galvan, A. Posada Amarillas, S. Mejía, C. Wing and M. José-Yacamán, en: J. M. Seminario (ed.), *Design and Applications of Nanomaterials for Sensors*, Challenges and Advances in Computational Chemistry and Physics 16, DOI 10.1007/978-94-017-8848-9\_10, © Springer Science+Business Media Dordrecht 2014.

## Copyright Registration

- Software BHUoS - Registro Público del Derecho de Autor No: 03-2016-031811504700-01
- Software NANOstructure - Registro Público del Derecho de Autor No: 03-2016-031811521300-01
- Software GenesUS - Registro Público del Derecho de Autor No: 03-2016-031811485600-01

## Patents

"Método de síntesis de nanopartículas de sulfuro de cobre", Alvaro Posada Amarillas, José Ronaldo Herrera Urbina, Instituto Mexicano de la Propiedad Industrial. File: MX/a/2012/006766. Jun 2012.

## Theses Supervisor

### B.Sc.

- "Cálculo ab initio del gap en halogenuros alcalinos", Margarita Franco-Ortiz, Feb 2004. Universidad de Sonora.
- "Propiedades estructurales y estabilidad en cúmulos de oro, plata y cobre", Johann Omar Zazueta-Sánchez, Jun 2005. Universidad de Sonora.
- "Cálculos DFT en dímeros de metales nobles y de transición", Alvaro Posada Borbón, Dic 2013. Universidad de Sonora.



- “Síntesis de nanopartículas metálicas con extracto de té verde: caracterización física y biológica”, Mario Alberto García Soqui, Jun 2016. Universidad de Sonora

#### **M.Sc.**

- "Estudio Teórico-Experimental de la densidad de estados electrónicos en la vecindad de la banda de conducción en cristales de  $\text{KCl:Cu}^+$  y  $\text{KCl:In}^{3+}$ ", Margarita Franco-Ortiz, Jun 2006. Universidad de Sonora.
- “Estudio de propiedades electrónicas y estructurales mediante método Kohn-Sham DFT para nanoaleaciones de 13 átomos de  $\text{Pd}_n\text{-Pt}_m$  “, Maribel Dessens-Félix, Nov 2009. Universidad de Sonora.
- "Computational modelling of nanoalloys", Josafat Guerrero Jordan, Maestría en Ciencias (Física), Dec., 2012. Co-Supervised by Prof. Roy L. Johnston.

#### **Dr.**

- "Cálculo de propiedades estructurales y dinámicas de metales líquidos por medio de simulación computacional", Efraín Urrutia-Bañuelos, Jun 2003. Universidad de Sonora.
- "Determinación de los mecanismos de formación de nanopartículas de plata sintetizadas en etilén glicol utilizando caracterización teórica y experimental de la banda del plasmón", Ángel Slistan-Grijalva, Apr 2005. Universidad de Sonora.
- “Paisaje de energía de nanopartículas bimetálicas”, Rafael Pacheco-Contreras, Jun 2010. Universidad de Sonora.
- “Estudio teórico de estabilidad estructural en nanopartículas bimetálicas”, Maribel Dessens Félix, Nov 2014. Universidad de Sonora.
- "Síntesis y caracterización de nanopartículas de sulfuro de cobre obtenidas por el método poliol", Jesús Humberto Coronado López, Nov 2015. Universidad de Sonora.
- "Estudios quimicocuánticos de nanopartículas semiconductoras en fase gas", José Octavio Juárez Sánchez, Nov 2015. Universidad de Sonora.