Curriculum Vitae - Dr. Alvaro Posada-Amarillas

PERSONAL DETAILS

NAME: Alvaro Posada-Amarillas

INSTITUTION: Department of Research in Physics, Universidad de Sonora

TITLE: Full-time Researcher

CONTACT DETAILS:

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

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

UNIVERSITY EDUCATION

Dr. PHYSICS OF MATERIALS Jan 1992-Jul 1996	Centro de Investigación Científica y de Educación Superior de Ensenada, Ensenada, B.C., México
M.Sc. PHYSICS Aug 1985-Jul 1987	Departamento de Investigación en Física, Universidad de Sonora, Hermosillo, Sonora, México.
B.Sc. PHYSICS Jan 1980-Jun 1985	Departamento de Física, Universidad de Sonora, Hermosillo, Sonora, 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, 2013-2015.

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 characterization; supported sub-nano clusters.

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_n clusters", Alvaro Posada-Amarillas and Ignacio L. Garzón, *Physical Review B* **54**, 10362(1996).

- "Structural and vibrational analysis of amorphous Au_{55} 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_{38} 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. Castillón 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 $YbFe_4Sb_{12}$, UFe_4P_{12}, and $ThFe_4P_{12}$", 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 $CoSi_2$ and $NiSi_2$", 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. Castillón-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. Castillón-Barraza, A. Posada-Amarillas, *Physica E* **27**, 104-112 (2005).

- "Theoretical study of the electronic properties of PrM_2B_2C (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. Castillón-Barraza, A. Posada-Amarillas, *Materials Research Bulletin* **43**, 90 (2008).
- "Structure and stability of In_X^Z ($X \leq 9$; 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_xGa_{1-x} and $In_xGa_{1-x}N$", 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_2 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 $Pt@Pd_{12}$", 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 $NiSi_2$", 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. Castillón-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_1Pd_{12} 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_4 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. Castillón-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 $(CuS)_N$ 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 $Pd_{12}Pt_1$ 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 $Pt_{101-x}Au_x$ 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_{2+x} Nanoplatelets", D. H. Galvan, A. Posada-Amarillas, N. Elizondo, M. José-Yacamán, *Modern Research in Catalysis* **2**, 164-171 (2013).
- "Global Minimum $Pt_{13}M_{20}$ (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).

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.

M.Sc.

- "Estudio Teórico-Experimental de la densidad de estados electrónicos en la vecindad de la banda de conducción en cristales de KCl:Cu^{+} y KCl:In^{+}", 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 $Pd_{n-m}Pt_m$ ", 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.