# Miguel Fuentes-Cabrera

List of Publications by Year
in descending order



| 77 | 2,144 | 218677 | 243625 |
|---|---|---|---|
| papers | citations | 26 h-index | 44 g-index |

| 81 | 81 | 81 | 2887 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Bridge structure for the graphene/Ni(111) system: A first principles study. Physical Review B, 2008, 77, . | 3.2 | 158 |
| 2 | Dynamic Defrosting on Nanostructured Superhydrophobic Surfaces. Langmuir, 2013, 29, 9516-9524. | 3.5 | 158 |
| 3 | Electronic structure and properties of isoreticular metal-organic frameworks: The case of M-IRMOF1 (M=Zn, Cd, Be, Mg, and Ca). Journal of Chemical Physics, 2005, 123, 124713. | 3.0 | 147 |
| 4 | Atomicâ€Ł evel Sculpting of Crystalline Oxides: Toward Bulk Nanofabrication with Single Atomic Plane Precision. Small, 2015, 11, 5895-5900. | 10.0 | 73 |
| 5 | Molecular dynamics study of the dewetting of copper on graphite and graphene: Implications for nanoscale self-assembly. Physical Review E, 2011, 83, 041603. | 2.1 | 68 |
| 6 | Size-Expanded DNA Bases:Â An Ab Initio Study of Their Structural and Electronic Properties. Journal of Physical Chemistry B, 2005, 109, 21135-21139. | 2.6 | 64 |
| 7 | Supramolecular Self-Assembly of Ï€-Conjugated Hydrocarbons via 2D Cooperative CH/Ï€ Interaction. ACS Nano, 2012, 6, 566-572. | 14.6 | 63 |
| 8 | Heterohexamers Formed by CcmK3 and CcmK4 Increase the Complexity of Beta Carboxysome Shells. Plant Physiology, 2019, 179, 156-167. | 4.8 | 61 |
| 9 | Characterization of the tunneling conductance across DNA bases. Physical Review E, 2006, 74, 011919. | 2.1 | 58 |
| 10 | Engineering the Bacterial Microcompartment Domain for Molecular Scaffolding Applications. Frontiers in Microbiology, 2017, 8, 1441. | 3.5 | 57 |
| 11 | Theoretical Study on the Structure, Stability, and Electronic Properties of the Guanineâ^'Znâ^'Cytosine Base Pair in M-DNA. Journal of Physical Chemistry B, 2007, 111, 870-879. | 2.6 | 55 |
| 12 | Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258. | 2.5 | 52 |
| 13 | First-Principles Transversal DNA Conductance Deconstructed. Biophysical Journal, 2006, 91, L04-L06. | 0.5 | 51 |
| 14 | Size-Expanded yDNA Bases:Â An Ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 6379-6384. | 2.6 | 49 |
| 15 | The application of approximate density functionals to complex systems. International Journal of Quantum Chemistry, 1998, 69, 327-340. | 2.0 | 46 |
| 16 | Direct atomic fabrication and dopant positioning in Si using electron beams with active real-time image-based feedback. Nanotechnology, 2018, 29, 255303. | 2.6 | 46 |
| 17 | Formamide-Based Prebiotic Synthesis of Nucleobases: A Kinetically Accessible Reaction Route. Journal of Physical Chemistry A, 2012, 116, 720-726. | 2.5 | 44 |
| 18 | Self-assembly directed one-step synthesis of [4]radialene on Cu(100) surfaces. Nature Communications, 2018, 9, 3113. | 12.8 | 41 |

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|---|---|---|---|
| 19 | Evaluation of functionalized isoreticular metal organic frameworks (IRMOFs) as smart nanoporous preconcentrators of RDX. Sensors and Actuators B: Chemical, 2010, 148, 459-468. | 7.8 | 38 |
| 20 | Molecular dynamics simulations of the d(CCAACGTTGG)2 decamer in crystal environment: Comparison of atomic point-charge, extra-point, and polarizable force fields. Journal of Chemical Physics, 2004, 121, 6998-7008. | 3.0 | 36 |
| 21 | Theoretical Study on the Factors Controlling the Stability of the Borate Complexes of Ribose, Arabinose, Lyxose, and Xylose. Chemistry - A European Journal, 2008, 14, 9990-9998. | 3.3 | 34 |
| 22 | Electronic Structure of xDNA. Journal of Physical Chemistry B, 2007, 111, 9057-9061. | 2.6 | 31 |
| 23 | A Microfluidics and Agent-Based Modeling Framework for Investigating Spatial Organization in Bacterial Colonies: The Case of Pseudomonas Aeruginosa and H1-Type VI Secretion Interactions. Frontiers in Microbiology, 2018, 9, 33. | 3.5 | 30 |
| 24 | Controlling the Velocity of Jumping Nanodroplets Via Their Initial Shape and Temperature. ACS Nano, 2011, 5, 7130-7136. | 14.6 | 29 |
| 25 | Prebiotic Routes to Nucleosides: A Quantum Chemical Insight into the Energetics of the Multistep Reaction Pathways. Chemistry - A European Journal, 2011, 17, 847-854. | 3.3 | 29 |
| 26 | Molecular simulations of adsorption and diffusion of RDX in IRMOF-1. Molecular Simulation, 2009, 35, 910-919. | 2.0 | 28 |
| 27 | Nonlinear pressure dependence of the direct band gap in adamantine ordered-vacancy compounds. Physical Review B, 2010, 81, . | 3.2 | 27 |
| 28 | Effect of Charge Distribution on RDX Adsorption in IRMOF-10. Langmuir, 2010, 26, 5942-5950. | 3.5 | 27 |
| 29 | Theoretical study of the ordered-vacancy semiconducting compound CdAl2Se4. Journal of Physics Condensed Matter, 2001, 13, 1669-1684. | 1.8 | 26 |
| 30 | Competition between Collapse and Breakup in Nanometer-Sized Thin Rings Using Molecular Dynamics and Continuum Modeling. Langmuir, 2012, 28, 13960-13967. | 3.5 | 25 |
| 31 | Electronic Control over Attachment and Self-Assembly of Alkyne Groups on Gold. ACS Nano, 2012, 6, 9267-9275. | 14.6 | 25 |
| 32 | An Evaluation of Molecular Dynamics Performance on the Hybrid Cray XK6 Supercomputer. Procedia Computer Science, 2012, 9, 186-195. | 2.0 | 24 |
| 33 | Ab initiostudy of the vibrational and electronic properties of CdGa2S4and CdGa2Se4under pressure. Journal of Physics Condensed Matter, 2001, 13, 10117-10124. | 1.8 | 23 |
| 34 | Ab Initio Study of Naphtho-Homologated DNA Bases. Journal of Physical Chemistry B, 2008, 112, 2179-2186. | 2.6 | 23 |
| 35 | On the Stabilization of Ribose by Silicate Minerals. Astrobiology, 2011, 11, 115-121. | 3.0 | 23 |
| 36 | Self-Organized and Cu-Coordinated Surface Linear Polymerization. Scientific Reports, 2013, 3, 2102. | 3.3 | 23 |

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| 37 | Ultrahigh Conductivity in Two-Dimensional InSe via Remote Doping at Room Temperature. Journal of Physical Chemistry Letters, 2018, 9, 3897-3903. | 4.6 | 23 |
| 38 | Theoretical Study of the Initial Stages of Self-Assembly of a Carboxysomeâ€™s Facet. ACS Nano, 2016, 10, 5751-5758. | 14.6 | 19 |
| 39 | Coexistence of spinodal instability and thermal nucleation in thin-film rupture: Insights from molecular levels. Physical Review E, 2014, 89, 032403. | 2.1 | 18 |
| 40 | Aromaticity-induced changes in electronic properties of size-expanded DNA bases: Case of xC. International Journal of Quantum Chemistry, 2006, 106, 2339-2346. | 2.0 | 17 |
| 41 | Structural, Dynamical, and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases. Journal of Physical Chemistry A, 2011, 115, 11344-11354. | 2.5 | 16 |
| 42 | Signatures of the Rayleighâ€Plateau Instability Revealed by Imposing Synthetic Perturbations on Nanometerâ€Sized Liquid Metals on Substrates. Angewandte Chemie - International Edition, 2012, 51, 8768-8772. | 13.8 | 16 |
| 43 | Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine. Journal of Physical Chemistry B, 2009, 113, 14465-14472. | 2.6 | 15 |
| 44 | Principles of Design for Substrate-Supported Molecular Switches Based on Physisorbed and Chemisorbed States. ACS Applied Materials & Interfaces, 2018, 10, 26772-26780. | 8.0 | 15 |
| 45 | Reactive solid-state dewetting of Cuâ€“Ni films on silicon. Applied Physics Letters, 2010, 97, 253101. | 3.3 | 14 |
| 46 | Theoretical study of graphitic analogues of simple semiconductors. Modelling and Simulation in Materials Science and Engineering, 1999, 7, 929-938. | 2.0 | 13 |
| 47 | Phase stability and pressure-induced semiconductor to metal transition in crystalline GeSe2. Journal of Physics Condensed Matter, 2002, 14, 9589-9600. | 1.8 | 13 |
| 48 | Theoretical Studies on the Intermolecular Interactions of Potentially Primordial Baseâ€Pair Analogues. Chemistry - A European Journal, 2010, 16, 3057-3065. | 3.3 | 13 |
| 49 | Enhancing Enantiomeric Separation with Strain: The Case of Serine on Cu(531). Journal of the American Chemical Society, 2017, 139, 8167-8173. | 13.7 | 12 |
| 50 | Molecular simulations of adsorption of RDX and TATP on IRMOF-1(Be). Journal of Molecular Modeling, 2012, 18, 3363-3378. | 1.8 | 11 |
| 51 | Theoretical study of the structural, electronic and vibrational properties of CdIn2Te4. Thin Solid Films, 2000, 373, 19-22. | 1.8 | 9 |
| 52 | Theoretical modeling on the kinetics of the arsenate-ester hydrolysis: implications to the stability of As-DNA. Physical Chemistry Chemical Physics, 2011, 13, 10869. | 2.8 | 9 |
| 53 | On the Geometry and Electronic Structure of the As-DNA Backbone. Journal of Physical Chemistry Letters, 2011, 2, 389-392. | 4.6 | 9 |
| 54 | Iron Particle Nanodrilling of Few Layer Graphene at Low Electron Beam Accelerating Voltages. Particle and Particle Systems Characterization, 2013, 30, 76-82. | 2.3 | 9 |

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|---|---|---|---|
| 55 | Visualizing in Vivo Dynamics of Designer Nanoscaffolds. Nano Letters, 2020, 20, 208-217. | 9.1 | 9 |
| 56 | Benzo-homologated nucleobases in a nanotube-electrode set-up for DNA sequencing. Nanotechnology, 2007, 18, 424019. | 2.6 | 8 |
| 57 | Energetics of hydrogen storage in organolithium nanostructures. Chemical Physics Letters, 2007, 436, 150-154. | 2.6 | 8 |
| 58 | Dynamical Treatment of Charge Transfer through Duplex Nucleic Acids Containing Modified Adenines. ACS Nano, 2013, 7, 9396-9406. | 14.6 | 8 |
| 59 | Reply to â€œComment on â€˜Characterization of the tunneling conductance across DNA basesâ€™ â€• Physical Review E, 2007, 76, 013902. | 2.1 | 7 |
| 60 | Surface, Interface, and Temperature Effects on the Phase Separation and Nanoparticle Self Assembly of Bi-Metallic Ni0.5Ag0.5: A Molecular Dynamics Study. Nanomaterials, 2019, 9, 1040. | 4.1 | 7 |
| 61 | Toward Electronic Conductance Characterization of DNA Nucleotide Bases. Solid State Phenomena, 2007, 121-123, 1387-1390. | 0.3 | 6 |
| 62 | Atomic Edge-Guided Polyethylene Crystallization on Monolayer Two-Dimensional Materials. Macromolecules, 2022, 55, 559-567. | 4.8 | 6 |
| 63 | Extrapolating Dynamic Leidenfrost Principles to Metallic Nanodroplets on Asymmetrically Textured Surfaces. Scientific Reports, 2015, 5, 11769. | 3.3 | 5 |
| 64 | Supramolecular polymerization of a prebiotic nucleoside provides insights into the creation of sequence-controlled polymers. Scientific Reports, 2016, 6, 18891. | 3.3 | 5 |
| 65 | Large Enantiospecificity of Stepâ€“kink Metal Surfaces: Contributions from the Backbone and Side Chain of Î±-Amino Acids. Journal of Physical Chemistry C, 2020, 124, 742-748. | 3.1 | 5 |
| 66 | Application of Machine Learning Techniques to an Agent-Based Model of Pantoea. Frontiers in Microbiology, 2021, 12, 726409. | 3.5 | 5 |
| 67 | External strain-enhanced cysteine enantiomeric separation ability on alloyed stepped surfaces. Journal of Chemical Physics, 2019, 150, 154701. | 3.0 | 4 |
| 68 | The Role of Phase Separation on Rayleigh-Plateau Type Instabilities in Alloys. Journal of Physical Chemistry C, 2021, 125, 5723-5731. | 3.1 | 4 |
| 69 | Electronic states of prototype supertetrahedral framework materials. Physical Review B, 2002, 66, . | 3.2 | 3 |
| 70 | Advancing Understanding and Design of Functional Materials Through Theoretical and Computational Chemical Physics. , 2012, , 209-278. | | 3 |
| 71 | Self-Propulsion Enhances Polymerization. Entropy, 2020, 22, 251. | 2.2 | 3 |
| 72 | Patterning: Atomicâ€Level Sculpting of Crystalline Oxides: Toward Bulk Nanofabrication with Single Atomic Plane Precision (Small 44/2015). Small, 2015, 11, 5854-5854. | 10.0 | 2 |

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| 73 | Isomeric effects on the self-assembly of a plausible prebiotic nucleoside analogue: A theoretical study. International Journal of Quantum Chemistry, 2017, 117, 213-221. | 2.0 | 2 |
| 74 | Ab-initio Study of the Diffusion Coefficients in Fe-based Liquids. Materials Research Society Symposia Proceedings, 2003, 806, 155. | 0.1 | 1 |
| 75 | Electronic and Structural High Pressure Properties of CuGaS 2 Chalcopyrite Semiconductor. High Pressure Research, 2002, 22, 361-364. | 1.2 | 0 |
| 76 | Nanodrilling: Iron Particle Nanodrilling of Few Layer Graphene at Low Electron Beam Accelerating Voltages (Part. Part. Syst. Charact. 1/2013). Particle and Particle Systems Characterization, 2013, 30, 75-75. | 2.3 | 0 |
| 77 | Theoretical and experimental evidence of conformational transformation in stereoisomers of nucleoside analogues. International Journal of Quantum Chemistry, 2018, 118, e25714. | 2.0 | 0 |