# Jose Javier Plata Ramos

List of Publications by Year
in descending order

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Version: 2024-02-01

| 42 | 2,207 | 331670 21 | 330143 37 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 44 | 44 | 44 | 3468 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Charting the Lattice Thermal Conductivities of Iâ€“IIIâ€“VI<sub>2</sub> Chalcopyrite Semiconductors. Chemistry of Materials, 2022, 34, 2833-2841. | 6.7 | 22 |
| 2 | Connecting experimental synthetic variables with the microstructure and electronic properties of doped ferroelectric perovskites for solar cell applications using high-throughput frameworks. Acta Materialia, 2021, 204, 116466. | 7.9 | 4 |
| 3 | High-Throughput Screening of the Thermoelastic Properties of Ultrahigh-Temperature Ceramics. ACS Applied Materials & Interfaces, 2021, 13, 29843-29857. | 8.0 | 8 |
| 4 | The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812. | | 4 |
| 5 | Understanding the Photocatalytic Properties of Pt/CeO<sub>x</sub>/TiO<sub>2</sub>: Structural Effects on Electronic and Optical Properties. ChemPhysChem, 2019, 20, 1624-1629. | 2.1 | 8 |
| 6 | The AFLOW Fleet for Materials Discovery. , 2019, , 1-28. | | 0 |
| 7 | Photo-sensitizing thin-film ferroelectric oxides using materials databases and high-throughput calculations. Journal of Materials Chemistry A, 2019, 7, 27323-27333. | 10.3 | 12 |
| 8 | Spinodal Superlattices of Topological Insulators. Chemistry of Materials, 2018, 30, 2331-2340. | 6.7 | 8 |
| 9 | The AFLOW Fleet for Materials Discovery. , 2018, , 1-28. | | 9 |
| 10 | Analysis of the variables that modify the robustness of Ti-SiO2 catalysts for alkene epoxidation: Role of silylation, deactivation and potential solutions. Molecular Catalysis, 2018, 459, 55-60. | 2.0 | 9 |
| 11 | Improving the activity of gold nanoparticles for the water-gas shift reaction using TiO<sub>2</sub>â€“Y<sub>2</sub>O<sub>3</sub>: an example of catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 22076-22083. | 2.8 | 8 |
| 12 | Effects of the capping ligands, linkers and oxide surface on the electron injection mechanism of copper sulfide quantum dot-sensitized solar cells. Physical Chemistry Chemical Physics, 2017, 19, 14580-14587. | 2.8 | 12 |
| 13 | An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOWâ€”AAPL Automatic Anharmonic Phonon Library. Npj Computational Materials, 2017, 3, . | 8.7 | 65 |
| 14 | Ag<sub>2</sub>S Quantum Dot-Sensitized Solar Cells by First Principles: The Effect of Capping Ligands and Linkers. Journal of Physical Chemistry A, 2017, 121, 7290-7296. | 2.5 | 17 |
| 15 | High throughput combinatorial method for fast and robust prediction of lattice thermal conductivity. Scripta Materialia, 2017, 129, 88-93. | 5.2 | 40 |
| 16 | Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screen thermomechanical properties of solids. Physical Review Materials, 2017, 1, . | 2.4 | 47 |
| 17 | High-throughput prediction of finite-temperature properties using the quasi-harmonic approximation. Computational Materials Science, 2016, 125, 82-91. | 3.0 | 51 |
| 18 | Cu Deposited on CeOx-Modified TiO<sub>2</sub>(110): Synergistic Effects at the Metalâ€“Oxide Interface and the Mechanism of the WGS Reaction. ACS Catalysis, 2016, 6, 4608-4615. | 11.2 | 43 |

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|---|---|---|---|
| 19 | First principles thermodynamical modeling of the binodal and spinodal curves in lead chalcogenides. Physical Chemistry Chemical Physics, 2016, 18, 5005-5011. | 2.8 | 13 |
| 20 | Structural, electronic and optical properties of copper, silver and gold sulfide: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1. | 1.4 | 35 |
| 21 | The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238. | 3.0 | 244 |
| 22 | Charting the complete elastic properties of inorganic crystalline compounds. Scientific Data, 2015, 2, 150009. | 5.3 | 642 |
| 23 | High-throughput computational screening of thermal conductivity, Debye temperature, and GrÃ¼neisen parameter using a quasiharmonic Debye model. Physical Review B, 2014, 90, . | 3.2 | 230 |
| 24 | Surface oxygen vacancies in gold based catalysts for CO oxidation. RSC Advances, 2014, 4, 13145-13152. | 3.6 | 24 |
| 25 | Understanding the Interplay of Dopants, Interfaces, and Anionic Conductivity in Doped Ceria/Zirconia Heteroepitaxial Structures. Chemistry of Materials, 2014, 26, 3385-3390. | 6.7 | 16 |
| 26 | Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Highlights in Theoretical Chemistry, 2014, , 177-183. | 0.0 | 0 |
| 27 | Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Theoretical Chemistry Accounts, 2013, 132, 1. | 1.4 | 5 |
| 28 | Nature of the Mixed-Oxide Interface in Ceriaâ€“Titania Catalysts: Clusters, Chains, and Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 14463-14471. | 3.1 | 73 |
| 29 | Electron Mobility via Polaron Hopping in Bulk Ceria: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 14502-14509. | 3.1 | 75 |
| 30 | Effect of structure and size on the excited states dynamics of CaArn clusters. European Physical Journal D, 2013, 67, 1. | 1.3 | 5 |
| 31 | Transport Properties in the CeO<sub>2â€“x</sub>(111) Surface: From Charge Distribution to Ion-Electron Collaborative Migration. Journal of Physical Chemistry C, 2013, 117, 25497-25503. | 3.1 | 41 |
| 32 | Making Photo-selective TiO<sub>2</sub> Materials by Cationâ€“Anion Codoping: From Structure and Electronic Properties to Photoactivity. Journal of Physical Chemistry C, 2012, 116, 18759-18767. | 3.1 | 29 |
| 33 | Ceria(100) Nanotubes with Negative Strain Energy: A First-Principles Prediction. Journal of Physical Chemistry Letters, 2012, 3, 2092-2096. | 4.6 | 5 |
| 34 | Communication: Improving the density functional theory+U description of CeO2 by including the contribution of the O 2p electrons. Journal of Chemical Physics, 2012, 136, 041101. | 3.0 | 62 |
| 35 | Understanding Acetaldehyde Thermal Chemistry on the TiO<sub>2</sub> (110) Rutile Surface: From Adsorption to Reactivity. Journal of Physical Chemistry C, 2011, 115, 2819-2825. | 3.1 | 22 |
| 36 | Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO<sub>2</sub>and Ce<sub>2</sub>O<sub>3</sub>. Journal of Chemical Theory and Computation, 2011, 7, 56-65. | 5.3 | 125 |

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|---|---|---|---|
| 37 | Structural Defects in W-Doped TiO<sub>2</sub> (101) Anatase Surface: Density Functional Study. Journal of Physical Chemistry C, 2011, 115, 16970-16976. | 3.1 | 34 |
| 38 | Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity. Topics in Catalysis, 2011, 54, 219-228. | 2.8 | 25 |
| 39 | A theoretical insight into the catalytic effect of a mixed-metal oxide at the nanometer level: The case of the highly active metal/CeOx/TiO2(110) catalysts. Journal of Chemical Physics, 2010, 132, 104703. | 3.0 | 93 |
| 40 | Vinyl Acetate Synthesis on Homogeneous and Heterogeneous Pd-Based Catalysts: A Theoretical Analysis on the Reaction Mechanisms. Journal of Physical Chemistry A, 2009, 113, 11758-11762. | 2.5 | 13 |
| 41 | Role of Coverage and Surface Oxidation Degree in the Adsorption of Acetone on TiO<sub>2</sub>(110). A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 19973-19980. | 3.1 | 24 |
| 42 | Machine Learning Approaches for Accelerating the Discovery of Thermoelectric Materials. ACS Symposium Series, 0, , 1-32. | 0.5 | 5 |