Jose Javier Plata Ramos

List of Publications by Year
in descending order

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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 complete elastic properties of inorganic crystalline compounds. Scientific Data, 2015, 2, 150009.	5.3	642
2	The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238.	3.0	244
3	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
4	Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO₂and Ce₂O₃. Journal of Chemical Theory and Computation, 2011, 7, 56-65.	5.3	125
5	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
6	Electron Mobility via Polaron Hopping in Bulk Ceria: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 14502-14509.	3.1	75
7	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
8	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
9	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
10	High-throughput prediction of finite-temperature properties using the quasi-harmonic approximation. Computational Materials Science, 2016, 125, 82-91.	3.0	51
11	Combining the AFLOW GIBBS and elastic libraries to efficiently and robustly screen thermomechanical properties of solids. Physical Review Materials, 2017, 1, .	2.4	47
12	Cu Deposited on CeOx-Modified TiO₂(110): Synergistic Effects at the Metalâ€“Oxide Interface and the Mechanism of the WGS Reaction. ACS Catalysis, 2016, 6, 4608-4615.	11.2	43
13	Transport Properties in the CeO_{2â€“x}(111) Surface: From Charge Distribution to Ion-Electron Collaborative Migration. Journal of Physical Chemistry C, 2013, 117, 25497-25503.	3.1	41
14	High throughput combinatorial method for fast and robust prediction of lattice thermal conductivity. Scripta Materialia, 2017, 129, 88-93.	5.2	40
15	Structural, electronic and optical properties of copper, silver and gold sulfide: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	35
16	Structural Defects in W-Doped TiO₂ (101) Anatase Surface: Density Functional Study. Journal of Physical Chemistry C, 2011, 115, 16970-16976.	3.1	34
17	Making Photo-selective TiO₂ Materials by Cationâ€“Anion Codoping: From Structure and Electronic Properties to Photoactivity. Journal of Physical Chemistry C, 2012, 116, 18759-18767.	3.1	29
18	Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity. Topics in Catalysis, 2011, 54, 219-228.	2.8	25

#	Article	IF	Citations
19	Role of Coverage and Surface Oxidation Degree in the Adsorption of Acetone on TiO₂(110). A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 19973-19980.	3.1	24
20	Surface oxygen vacancies in gold based catalysts for CO oxidation. RSC Advances, 2014, 4, 13145-13152.	3.6	24
21	Understanding Acetaldehyde Thermal Chemistry on the TiO₂ (110) Rutile Surface: From Adsorption to Reactivity. Journal of Physical Chemistry C, 2011, 115, 2819-2825.	3.1	22
22	Charting the Lattice Thermal Conductivities of Iâ€“IIIâ€“VI₂ Chalcopyrite Semiconductors. Chemistry of Materials, 2022, 34, 2833-2841.	6.7	22
23	Ag₂S 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
24	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
25	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
26	First principles thermodynamical modeling of the binodal and spinodal curves in lead chalcogenides. Physical Chemistry Chemical Physics, 2016, 18, 5005-5011.	2.8	13
27	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
28	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
29	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
30	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
31	Spinodal Superlattices of Topological Insulators. Chemistry of Materials, 2018, 30, 2331-2340.	6.7	8
32	Improving the activity of gold nanoparticles for the water-gas shift reaction using TiO₂â€“Y₂O₃: an example of catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 22076-22083.	2.8	8
33	Understanding the Photocatalytic Properties of Pt/CeO_x/TiO₂: Structural Effects on Electronic and Optical Properties. ChemPhysChem, 2019, 20, 1624-1629.	2.1	8
34	High-Throughput Screening of the Thermoelastic Properties of Ultrahigh-Temperature Ceramics. ACS Applied Materials & Interfaces, 2021, 13, 29843-29857.	8.0	8
35	Ceria(100) Nanotubes with Negative Strain Energy: A First-Principles Prediction. Journal of Physical Chemistry Letters, 2012, 3, 2092-2096.	4.6	5
36	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

#	Article	IF	Citations
37	Effect of structure and size on the excited states dynamics of CaArn clusters. European Physical Journal D, 2013, 67, 1.	1.3	5
38	Machine Learning Approaches for Accelerating the Discovery of Thermoelectric Materials. ACS Symposium Series, 0, , 1-32.	0.5	5
39	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
40	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
41	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0
42	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