Ricardo Grau-Crespo

List of Publications by Year
in descending order

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100 papers	3,138 citations	136950 32 h-index	175258 52 g-index
105 all docs	105 docs citations	105 times ranked	5065 citing authors

#	Article	IF	Citations
1	Mixed-anion mixed-cation perovskite (FAPbI₃)_{0.875}(MAPbBr₃)_{0.125}: an ab initio molecular dynamics study. Journal of Materials Chemistry A, 2022, 10, 9592-9603.	10.3	4
2	Charting the Lattice Thermal Conductivities of Iâ€“IIIâ€“VI₂ Chalcopyrite Semiconductors. Chemistry of Materials, 2022, 34, 2833-2841.	6.7	22
3	Distributed representations of atoms and materials for machine learning. Npj Computational Materials, 2022, 8, .	8.7	9
4	Bromate incorporation in calcite and aragonite. Geochimica Et Cosmochimica Acta, 2022, 324, 17-25.	3.9	2
5	Tin-Substituted Chalcopyrite: An n-Type Sulfide with Enhanced Thermoelectric Performance. Chemistry of Materials, 2022, 34, 5860-5873.	6.7	12
6	Interface chemistry effects in nanofluids: Experimental and computational study of oil-based nanofluids with gold nanoplates. Journal of Molecular Liquids, 2022, 362, 119762.	4.9	3
7	Tilt and shift polymorphism in molecular perovskites. Materials Horizons, 2021, 8, 2444-2450.	12.2	12
8	Linking in situ charge accumulation to electronic structure in doped SrTiO3 reveals design principles for hydrogen-evolving photocatalysts. Nature Materials, 2021, 20, 511-517.	27.5	82
9	Interfacial molecular layering enhances specific heat of nanofluids: Evidence from molecular dynamics. Journal of Molecular Liquids, 2021, 325, 115217.	4.9	30
10	Optical and Transport Properties of Metalâ€“Oil Nanofluids for Thermal Solar Industry: Experimental Characterization, Performance Assessment, and Molecular Dynamics Insights. ACS Sustainable Chemistry and Engineering, 2021, 9, 4194-4205.	6.7	10
11	Engineering the electronic and optical properties of 2D porphyrin-paddlewheel metal-organic frameworks. JPhys Energy, 2021, 3, 034005.	5.3	7
12	Polaron-Adsorbate Coupling at the TiO₂(110)-Carboxylate Interface. Journal of Physical Chemistry Letters, 2021, 12, 3571-3576.	4.6	14
13	Bandgap Engineering in the Configurational Space of Solid Solutions via Machine Learning: (Mg,Zn)O Case Study. Journal of Physical Chemistry Letters, 2021, 12, 5163-5168.	4.6	8
14	Sulfate and Molybdate Incorporation at the Calciteâ€“Water Interface: Insights from Ab Initio Molecular Dynamics. ACS Earth and Space Chemistry, 2021, 5, 2066-2073.	2.7	3
15	Intrinsic and extrinsic nature of the giant piezoelectric effect in the initial poling of PMN-PT. Physical Review Materials, 2021, 5, .	2.4	2
16	Molybdenum and sulfur incorporation as oxyanion substitutional impurities in calcium carbonate minerals: A computational investigation. Chemical Geology, 2020, 553, 119796.	3.3	8
17	Adsorption of Aspartic Acid on Ni{100}: A Combined Experimental and Theoretical Study. Langmuir, 2020, 36, 9399-9411.	3.5	5
18	Understanding the Specific Heat Enhancement in Metal-Containing Nanofluids for Thermal Energy Storage: Experimental and Ab Initio Evidence for a Strong Interfacial Layering Effect. ACS Applied Energy Materials, 2020, 3, 9246-9256.	5.1	20

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19	The closed-edge structure of graphite and the effect of electrostatic charging. RSC Advances, 2020, 10, 7994-8001.	3.6	12
20	Novel WS₂-Based Nanofluids for Concentrating Solar Power: Performance Characterization and Molecular-Level Insights. ACS Applied Materials & Interfaces, 2020, 12, 5793-5804.	8.0	22
21	Single-site binding of pyrene to poly(ester-imide)s incorporating long spacer-units: prediction of NMR resonance-patterns from a fractal model. Chemical Science, 2020, 11, 12165-12177.	7.4	1
22	Understanding the origin of disorder in kesterite-type chalcogenides A₂ZnBQ₄ (A = Cu, Ag; B = Sn, Ge; Q = S, Se): the influence of inter-layer interactions. Physical Chemistry Chemical Physics, 2019, 21, 19311-19317.	2.8	16
23	Ensemble-Based Modeling of the NMR Spectra of Solid Solutions: Cation Disorder in Y₂(Sn,Ti)₂O₇. Journal of the American Chemical Society, 2019, 141, 17838-17846.	13.7	29
24	Electron and phonon interactions and transport in the ultrahigh-temperature ceramic ZrC. Physical Review B, 2019, 99, .	3.2	12
25	Double-well potential energy surface in the interaction between h-BN and Ni(111). Physical Chemistry Chemical Physics, 2019, 21, 10888-10894.	2.8	7
26	Origin of the transition entropy in vanadium dioxide. Physical Review B, 2019, 99, .	3.2	20
27	Supramolecular complexation between chain-folding poly(ester-imide)s and polycyclic aromatics: a fractal-based pattern of NMR ring-current shielding. Polymer Chemistry, 2019, 10, 6641-6650.	3.9	3
28	Mixing Thermodynamics and Photocatalytic Properties of GaPâ€“ZnS solid solutions. Advanced Theory and Simulations, 2019, 2, 1800146.	2.8	7
29	Combined Experimental and Theoretical Study of Methyl Acetoacetate Adsorption on Ni{100}. Journal of Physical Chemistry C, 2018, 122, 6186-6194.	3.1	6
30	Operando spectroscopy study of the carbon dioxide electro-reduction by iron species on nitrogen-doped carbon. Nature Communications, 2018, 9, 935.	12.8	182
31	Origin of the monolayer Raman signature in hexagonal boron nitride: a first-principles analysis. Journal of Physics Condensed Matter, 2018, 30, 185701.	1.8	3
32	Elements of fractal geometry in the ¹H NMR spectrum of a copolymer intercalation-complex: identification of the underlying Cantor set. Chemical Science, 2018, 9, 4052-4061.	7.4	5
33	Band Structures of Periodic Porphyrin Nanostructures. Journal of Physical Chemistry C, 2018, 122, 23790-23798.	3.1	21
34	Screening heteroatom distributions in zeotype materials using an effective Hamiltonian approach: the case of aluminogermanate PKU-9. Physical Chemistry Chemical Physics, 2018, 20, 18047-18055.	2.8	3
35	Porphyrin-based metal-organic frameworks for solar fuel synthesis photocatalysis: band gap tuning via iron substitutions. Journal of Materials Chemistry A, 2017, 5, 11894-11904.	10.3	84
36	Unsupported trimetallic Ni(Co)-Mo-W sulphide catalysts prepared from mixed oxides: Characterisation and catalytic tests for simultaneous tetralin HDA and dibenzothiophene HDS reactions. Catalysis Today, 2017, 292, 84-96.	4.4	21

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37	Crystal structure of cobalt hydroxide carbonate Co₂CO₃(OH)₂: density functional theory and X-ray diffraction investigation. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 868-873.	1.1	12
38	Critical Role of Dynamic Flexibility in Geâ€Containing Zeolites: Impact on Diffusion. Chemistry - A European Journal, 2016, 22, 10036-10043.	3.3	22
39	Frontispiz: Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie, 2016, 128, .	2.0	0
40	Frontispiece: Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie - International Edition, 2016, 55, .	13.8	1
41	Quantitative Structure of an Acetate Dye Molecule Analogue at the TiO₂â€“Acetic Acid Interface. Journal of Physical Chemistry C, 2016, 120, 7586-7590.	3.1	7
42	Electron and phonon transport in shandite-structured<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Ni</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Sn</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2016, 94, .	3.2	12
43	Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie - International Edition, 2016, 55, 16012-16016.	13.8	61
44	Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie, 2016, 128, 16246-16250.	2.0	12
45	Adsorption of Methyl Acetoacetate at Ni{111}: Experiment and Theory. Journal of Physical Chemistry C, 2016, 120, 27490-27499.	3.1	17
46	Importance of anisotropic Coulomb interaction in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2015, 92, .	3.2	47
47	First-principles study of the inversion thermodynamics and electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Fe</mml:mi><mml:msub><mml:mi>M</mml:mi><mml:mi		

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55	Spin polarization, orbital occupation and band gap opening in vanadium dioxide: The effect of screened Hartreeâ€“Fock exchange. Chemical Physics Letters, 2014, 608, 126-129.	2.6	16
56	A Computational Study of Magnesium Incorporation in the Bulk and Surfaces of Hydroxyapatite. Langmuir, 2013, 29, 5851-5856.	3.5	17
57	Aluminium distribution in ZSM-5 revisited: The role of Alâ€“Al interactions. Journal of Solid State Chemistry, 2013, 198, 330-336.	2.9	21
58	Lithium and oxygen adsorption at the Î²-MnO2 (110) surface. Journal of Materials Chemistry A, 2013, 1, 14879.	10.3	58
59	Scanning Tunneling Microscopy and Molecular Dynamics Study of the Li₂TiO₃(001) Surface. Journal of Physical Chemistry C, 2013, 117, 5126-5131.	3.1	21
60	General model for explicitly hole-doped superconductor parent compounds: Electronic structure of Ca<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Na<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>CuO<mml:math xmlns:mml="http://www.w3.org/1998/M	3.2	5
61	Density functional theory study of rutile VO2 surfaces. Journal of Chemical Physics, 2012, 137, 154706.	3.0	69
62	Molecular Simulation of Wetting Transitions on Novel Materials. , 2012, , 235-258.		2
63	Band gap control via tuning of inversion degree in CdIn2S4 spinel. Applied Physics Letters, 2012, 100, .	3.3	31
64	Why the Heyd-Scuseria-Ernzerhof hybrid functional description of VO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>phases is not correct. Physical Review B, 2012, 86, .	3.2	68
65	Cation distribution and mixing thermodynamics in Fe/Ni thiospinels. Geochimica Et Cosmochimica Acta, 2012, 88, 275-282.	3.9	21
66	Mg/Ca Partitioning Between Aqueous Solution and Aragonite Mineral: A Molecular Dynamics Study. Chemistry - A European Journal, 2012, 18, 9828-9833.	3.3	10
67	Following the Creation of Active Gold Nanocatalysts from Phosphine-Stabilized Molecular Clusters. ACS Catalysis, 2012, 2, 957-963.	11.2	46
68	Introducing k-point parallelism into VASP. Computer Physics Communications, 2012, 183, 1696-1701.	7.5	33
69	Mixing Thermodynamics of the Calcite-Structured (Mn,Ca)CO₃ Solid Solution: A Computer Simulation Study. Journal of Physical Chemistry B, 2011, 115, 13854-13861.	2.6	35
70	The interplay between dopants and oxygen vacancies in the magnetism of V-doped TiO₂. Journal of Physics Condensed Matter, 2011, 23, 334216.	1.8	10
71	Substitutional and orientational disorder in organic crystals: a symmetry-adapted ensemble model. Physical Chemistry Chemical Physics, 2011, 13, 9590.	2.8	49
72	Phase separation and surface segregation in ceriaâ€“zirconia solid solutions. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 1925-1938.	2.1	45

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73	Dopant-vacancy binding effects in Li-doped magnesium hydride. Physical Review B, 2010, 82, .	3.2	27
74	Vacancy ordering and electronic structure of Î³-Fe₂O₃(maghemite): a theoretical investigation. Journal of Physics Condensed Matter, 2010, 22, 255401.	1.8	172
75	Electronic Structure and Redox Properties of the Ti-Doped Zirconia (111) Surface. Journal of Physical Chemistry C, 2010, 114, 15403-15409.	3.1	20
76	Thermochemistry of strontium incorporation in aragonite from atomistic simulations. Geochimica Et Cosmochimica Acta, 2010, 74, 1320-1328.	3.9	34
77	Electronic structure and magnetic ordering of the unconventional antiferromagnet Yb 3 Pt 4. Europhysics Letters, 2009, 88, 67001.	2.0	1
78	Thermodynamics of hydrogen vacancies in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgH</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms first-principles calculations and grand-canonical statistical mechanics. Physical Review B, 2009, 80, .	3.2	23
79	Redox properties of gold-substituted zirconia surfaces. Journal of Materials Chemistry, 2009, 19, 710-717.	6.7	12
80	Electronic and magnetic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>GGA</mml:mtext><mml:mo>+</mml:mo><mml:mtext>U</mml:mtext></mml:mrow></mml Physical Review B, 2009, 79, .	3.2	61
81	A theoretical investigation of Î±-Fe₂O₃â€“Cr₂O₃solid solutions. Physical Chemistry Chemical Physics, 2009, 11, 808-815.	2.8	51
82	On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO[sub 2](111). Journal of Chemical Physics, 2009, 131, 094702.	3.0	64
83	Electronic charge transfer between ceria surfaces and gold adatoms: a GGA+U investigation. Physical Chemistry Chemical Physics, 2009, 11, 5246.	2.8	83
84	Combined Density Functional Theory and Interatomic Potential Study of the Bulk and Surface Structures and Properties of the Iron Sulfide Mackinawite (FeS). Journal of Physical Chemistry C, 2008, 112, 10960-10967.	3.1	70
85	Redox Behavior of the Model Catalyst Pd/CeO2â^'x/Pt(111). Journal of Physical Chemistry C, 2008, 112, 10918-10922.	3.1	62
86	Theoretical Investigation of the Deposition of Cu, Ag, and Au Atoms on the ZrO2(111) Surface. Journal of Physical Chemistry C, 2007, 111, 10448-10454.	3.1	58
87	Symmetry-adapted configurational modelling of fractional site occupancy in solids. Journal of Physics Condensed Matter, 2007, 19, 256201.	1.8	182
88	A computer modeling study of redox processes on the FeSbO4 (100) surface. Journal of Catalysis, 2007, 248, 77-88.	6.2	17
89	The effect of cation coordination on the properties of oxygen vacancies in FeSbO4. Journal of Materials Chemistry, 2006, 16, 1943.	6.7	19
90	Electronic structure and magnetic coupling inFeSbO4: A DFT study using hybrid functionals andGGA+Umethods. Physical Review B, 2006, 73, .	3.2	43

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91	A computational study of the effect of Liâ€“K solid solutions on the structures and stabilities of layered silicate materialsâ€”an application of the use of Condor pools in molecular simulation. Molecular Simulation, 2005, 31, 339-347.	2.0	6
92	Distribution of Cations in FeSbO4: A Computer Modeling Study. Chemistry of Materials, 2004, 16, 1954-1960.	6.7	37
93	Cation distribution and magnetic ordering in FeSbO4. Journal of Materials Chemistry, 2003, 13, 2848.	6.7	42
94	A free energy minimisation study of the monoclinicâ€“orthorhombic transition in MFI zeolite. Chemical Communications, 2002, , 2544-2545.	4.1	28
95	Comment on â€œAb initio study of MoS2and Li adsorbed on the (101Ì„0) face of MoS2â€•by V. Alexiev, R. Prins and Th. Weber, Phys. Chem. Chem. Phys., 2000, 2, 1815, and â€œDFT study of MoS2and hydrogen adsorbed on the (101Ì„0) face of MoS2â€•by V. Alexiev, R. Prins and Th. Weber, Phys. Chem. Chem. Phys., 2001, 3, 5326. Physical Chemistry Chemical Physics, 2002, 4, 4078-4079.	2.8	3
96	A computer simulation study of distribution, structure and acid strength of active sites in H-ZSM-5 catalyst. Physical Chemistry Chemical Physics, 2000, 2, 5716-5722.	2.8	47
97	A theoretical investigation of Î±-Fe2O3â€“Cr2O3 solid solutions. , 0, .		1
98	On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO2(111). , 0, .		1
99	The symmetry-adapted configurational ensemble approach to the computer simulation of site-disordered solids. , 0, , .		3
100	Machine Learning Approaches for Accelerating the Discovery of Thermoelectric Materials. ACS Symposium Series, 0, , 1-32.	0.5	5