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	Symmetry-adapted configurational modelling of fractional site occupancy in solids. Journal of Physics Condensed Matter, 2007, 19, 256201.	1.8	182
2	Operando spectroscopy study of the carbon dioxide electro-reduction by iron species on nitrogen-doped carbon. Nature Communications, 2018, 9, 935.	12.8	182
3	A DFT study of the structures, stabilities and redox behaviour of the major surfaces of magnetite Fe₃O₄. Physical Chemistry Chemical Physics, 2014, 16, 21082-21097.	2.8	178
4	Vacancy ordering and electronic structure of Î³-Fe₂O₃(maghemite): a theoretical investigation. Journal of Physics Condensed Matter, 2010, 22, 255401.	1.8	172
5	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
6	Electronic charge transfer between ceria surfaces and gold adatoms: a GGA+U investigation. Physical Chemistry Chemical Physics, 2009, 11, 5246.	2.8	83
7	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
8	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><mml:m		

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19	Adsorption of organic molecules at the TiO2(110) surface: The effect of van der Waals interactions. Surface Science, 2015, 632, 142-153.	1.9	57
20	A theoretical investigation of Î±-Fe₂O₃â€“Cr₂O₃solid solutions. Physical Chemistry Chemical Physics, 2009, 11, 808-815.	2.8	51
21	Substitutional and orientational disorder in organic crystals: a symmetry-adapted ensemble model. Physical Chemistry Chemical Physics, 2011, 13, 9590.	2.8	49
22	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
23	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></ Physical Review B, 2015, 92, .	3.2	47
24	Interplay of Metal-Atom Ordering, Fermi Level Tuning, and Thermoelectric Properties in Cobalt Shandites Co₃M₂S₂ (M = Sn, In). Chemistry of Materials, 2015, 27, 3946-3956.	6.7	47
25	Following the Creation of Active Gold Nanocatalysts from Phosphine-Stabilized Molecular Clusters. ACS Catalysis, 2012, 2, 957-963.	11.2	46
26	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
27	Electronic structure and magnetic coupling inFeSbO4: A DFT study using hybrid functionals andGGA+Umethods. Physical Review B, 2006, 73, .	3.2	43
28	Cation distribution and magnetic ordering in FeSbO4. Journal of Materials Chemistry, 2003, 13, 2848.	6.7	42
29	Distribution of Cations in FeSbO4: A Computer Modeling Study. Chemistry of Materials, 2004, 16, 1954-1960.	6.7	37
30	Electronic Structure of Pd Multilayers on Re(0001): The Role of Charge Transfer. Journal of Physical Chemistry C, 2015, 119, 23436-23444.	3.1	37
31	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
32	Engineering the electronic bandgaps and band edge positions in carbon-substituted 2D boron nitride: a first-principles investigation. Physical Chemistry Chemical Physics, 2015, 17, 13547-13552.	2.8	35
33	Thermochemistry of strontium incorporation in aragonite from atomistic simulations. Geochimica Et Cosmochimica Acta, 2010, 74, 1320-1328.	3.9	34
34	Introducing k-point parallelism into VASP. Computer Physics Communications, 2012, 183, 1696-1701.	7.5	33
35	Band gap control via tuning of inversion degree in CdIn2S4 spinel. Applied Physics Letters, 2012, 100, .	3.3	31
36	Interfacial molecular layering enhances specific heat of nanofluids: Evidence from molecular dynamics. Journal of Molecular Liquids, 2021, 325, 115217.	4.9	30

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37	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
38	A free energy minimisation study of the monoclinicâ€“orthorhombic transition in MFI zeolite. Chemical Communications, 2002, , 2544-2545.	4.1	28
39	Dopant-vacancy binding effects in Li-doped magnesium hydride. Physical Review B, 2010, 82, .	3.2	27
40	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
41	Critical Role of Dynamic Flexibility in Geâ€Containing Zeolites: Impact on Diffusion. Chemistry - A European Journal, 2016, 22, 10036-10043.	3.3	22
42	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
43	Charting the Lattice Thermal Conductivities of Iâ€“IIIâ€“VI₂ Chalcopyrite Semiconductors. Chemistry of Materials, 2022, 34, 2833-2841.	6.7	22
44	Cation distribution and mixing thermodynamics in Fe/Ni thiospinels. Geochimica Et Cosmochimica Acta, 2012, 88, 275-282.	3.9	21
45	Aluminium distribution in ZSM-5 revisited: The role of Alâ€“Al interactions. Journal of Solid State Chemistry, 2013, 198, 330-336.	2.9	21
46	Scanning Tunneling Microscopy and Molecular Dynamics Study of the Li₂TiO₃(001) Surface. Journal of Physical Chemistry C, 2013, 117, 5126-5131.	3.1	21
47	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
48	Band Structures of Periodic Porphyrin Nanostructures. Journal of Physical Chemistry C, 2018, 122, 23790-23798.	3.1	21
49	Electronic Structure and Redox Properties of the Ti-Doped Zirconia (111) Surface. Journal of Physical Chemistry C, 2010, 114, 15403-15409.	3.1	20
50	Origin of the transition entropy in vanadium dioxide. Physical Review B, 2019, 99, .	3.2	20
51	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
52	The effect of cation coordination on the properties of oxygen vacancies in FeSbO4. Journal of Materials Chemistry, 2006, 16, 1943.	6.7	19
53	Cobalt incorporation in calcite: Thermochemistry of (Ca,Co)CO 3 solid solutions from density functional theory simulations. Geochimica Et Cosmochimica Acta, 2014, 142, 205-216.	3.9	18
54	A computer modeling study of redox processes on the FeSbO4 (100) surface. Journal of Catalysis, 2007, 248, 77-88.	6.2	17

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55	A Computational Study of Magnesium Incorporation in the Bulk and Surfaces of Hydroxyapatite. Langmuir, 2013, 29, 5851-5856.	3.5	17
56	Adsorption of Methyl Acetoacetate at Ni{111}: Experiment and Theory. Journal of Physical Chemistry C, 2016, 120, 27490-27499.	3.1	17
57	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
58	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
59	Polaron-Adsorbate Coupling at the TiO₂(110)-Carboxylate Interface. Journal of Physical Chemistry Letters, 2021, 12, 3571-3576.	4.6	14
60	Redox properties of gold-substituted zirconia surfaces. Journal of Materials Chemistry, 2009, 19, 710-717.	6.7	12
61	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
62	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
63	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
64	Electron and phonon interactions and transport in the ultrahigh-temperature ceramic ZrC. Physical Review B, 2019, 99, .	3.2	12
65	The closed-edge structure of graphite and the effect of electrostatic charging. RSC Advances, 2020, 10, 7994-8001.	3.6	12
66	Tilt and shift polymorphism in molecular perovskites. Materials Horizons, 2021, 8, 2444-2450.	12.2	12
67	Tin-Substituted Chalcopyrite: An n-Type Sulfide with Enhanced Thermoelectric Performance. Chemistry of Materials, 2022, 34, 5860-5873.	6.7	12
68	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
69	Mg/Ca Partitioning Between Aqueous Solution and Aragonite Mineral: A Molecular Dynamics Study. Chemistry - A European Journal, 2012, 18, 9828-9833.	3.3	10
70	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
71	Distributed representations of atoms and materials for machine learning. Npj Computational Materials, 2022, 8, .	8.7	9
72	Molybdenum and sulfur incorporation as oxyanion substitutional impurities in calcium carbonate minerals: A computational investigation. Chemical Geology, 2020, 553, 119796.	3.3	8

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73	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
74	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
75	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
76	Mixing Thermodynamics and Photocatalytic Properties of GaPâ€“ZnS solid solutions. Advanced Theory and Simulations, 2019, 2, 1800146.	2.8	7
77	Engineering the electronic and optical properties of 2D porphyrin-paddlewheel metal-organic frameworks. JPhys Energy, 2021, 3, 034005.	5.3	7
78	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
79	Combined Experimental and Theoretical Study of Methyl Acetoacetate Adsorption on Ni{100}. Journal of Physical Chemistry C, 2018, 122, 6186-6194.	3.1	6
80	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	3.2	5
81	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
82	Adsorption of Aspartic Acid on Ni{100}: A Combined Experimental and Theoretical Study. Langmuir, 2020, 36, 9399-9411.	3.5	5
83	Machine Learning Approaches for Accelerating the Discovery of Thermoelectric Materials. ACS Symposium Series, 0, , 1-32.	0.5	5
84	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
85	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
86	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
87	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
88	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
89	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
90	The symmetry-adapted configurational ensemble approach to the computer simulation of site-disordered solids. , 0, , .		3

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91	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
92	Molecular Simulation of Wetting Transitions on Novel Materials. , 2012, , 235-258.		2
93	Bromate incorporation in calcite and aragonite. Geochimica Et Cosmochimica Acta, 2022, 324, 17-25.	3.9	2
94	Intrinsic and extrinsic nature of the giant piezoelectric effect in the initial poling of PMN-PT. Physical Review Materials, 2021, 5, .	2.4	2
95	Electronic structure and magnetic ordering of the unconventional antiferromagnet Yb 3 Pt 4. Europhysics Letters, 2009, 88, 67001.	2.0	1
96	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
97	A theoretical investigation of Î±-Fe2O3â€“Cr2O3 solid solutions. , 0, .		1
98	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
99	On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO2(111). , 0, .		1
100	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