Alberto Otero de la Roza

List of Publications by Year
in descending order

103	9,834	136950 32	36028 97
papers	citations	h-index	g-index

107	107	107	11319
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A density-functional benchmark of vibrational free-energy corrections for molecular crystal polymorphism. Journal of Chemical Physics, 2022, 156, 114108.	3.0	7
2	Fast and Accurate Quantum Mechanical Modeling of Large Molecular Systems Using Small Basis Set Hartreeâ€“Fock Methods Corrected with Atom-Centered Potentials. Journal of Chemical Theory and Computation, 2022, 18, 2208-2232.	5.3	7
3	BH9, a New Comprehensive Benchmark Data Set for Barrier Heights and Reaction Energies: Assessment of Density Functional Approximations and Basis Set Incompleteness Potentials. Journal of Chemical Theory and Computation, 2022, 18, 151-166.	5.3	27
4	Small-Basis Set Density-Functional Theory Methods Corrected with Atom-Centered Potentials. Journal of Chemical Theory and Computation, 2022, 18, 2913-2930.	5.3	4
5	Phase stability and dense polymorph of the BaCa(CO3)2 barytocalcite carbonate. Scientific Reports, 2022, 12, 7413.	3.3	4
6	Finding critical points and reconstruction of electron densities on grids. Journal of Chemical Physics, 2022, 156, .	3.0	7
7	Experimental and computational evidence for a stabilising Câ€“Cl(lone-pair)â‹¯Ï€(chelate-ring) interaction. CrystEngComm, 2021, 23, 119-130.	2.6	4
8	Temperature and pressure-induced strains in anhydrous iron trifluoride polymorphs. Physical Chemistry Chemical Physics, 2021, 23, 2825-2835.	2.8	1
9	Controlling the off-center positions of anions through thermodynamics and kinetics in flexible perovskite-like materials. Physical Chemistry Chemical Physics, 2021, 23, 4491-4499.	2.8	2
10	Structural, vibrational and electronic properties of Î±â€²-Ga₂S₃ under compression. Physical Chemistry Chemical Physics, 2021, 23, 6841-6862.	2.8	8
11	Crystal Structure of BaCa(CO3)2 Alstonite Carbonate and Its Phase Stability upon Compression. ACS Earth and Space Chemistry, 2021, 5, 1130-1139.	2.7	11
12	Compressibility and Phase Stability of Iron-Rich Ankerite. Minerals (Basel, Switzerland), 2021, 11, 607.	2.0	7
13	Transition path to a dense efficient-packed post-delafossite phase. Crystal structure and evolution of the chemical bonding. Journal of Alloys and Compounds, 2021, 867, 159012.	5.5	1
14	Performance of small basis set Hartreeâ€“Fock methods for modeling non-covalent interactions. Electronic Structure, 2021, 3, 034007.	2.8	6
15	BSE49, a diverse, high-quality benchmark dataset of separation energies of chemical bonds. Scientific Data, 2021, 8, 300.	5.3	9
16	Experimental and Theoretical Study of SbPO4 under Compression. Inorganic Chemistry, 2020, 59, 287-307.	4.0	14
17	Analysis of Density-Functional Errors for Noncovalent Interactions between Charged Molecules. Journal of Physical Chemistry A, 2020, 124, 353-361.	2.5	5
18	Pressure and Temperature Effects on Low-Density Mg₃Ca(CO₃)₄ Huntite Carbonate. Journal of Physical Chemistry C, 2020, 124, 1077-1087.	3.1	11

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19	Application of XDM to ionic solids: The importance of dispersion for bulk moduli and crystal geometries. Journal of Chemical Physics, 2020, 153, 054121.	3.0	11
20	Interplay between local structure, vibrational and electronic properties on CuO under pressure. Physical Chemistry Chemical Physics, 2020, 22, 24299-24309.	2.8	3
21	Phase Stability of Natural Ni_{0.75}Mg_{0.22}Ca_{0.03}CO₃ Gaspeite Mineral at High Pressure and Temperature. Journal of Physical Chemistry C, 2020, 124, 19781-19792.	3.1	9
22	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
23	Improved Basis-Set Incompleteness Potentials for Accurate Density-Functional Theory Calculations in Large Systems. Journal of Chemical Theory and Computation, 2020, 16, 4176-4191.	5.3	15
24	Snap Frozen! Capturing Two Metastable Polymorphs in a Tetramorphic One-Dimensional Coordination Polymer Constructed from Cadmium, Dithiophosphate, and 4-Pyridinealdazine. Crystal Growth and Design, 2020, 20, 3272-3283.	3.0	8
25	Asymptotic Pairwise Dispersion Corrections Can Describe Layered Materials Accurately. Journal of Physical Chemistry Letters, 2020, 11, 2298-2302.	4.6	17
26	What is â€œmany-bodyâ€•dispersion and should I worry about it?. Physical Chemistry Chemical Physics, 2020, 22, 8266-8276.	2.8	30
27	Dispersion XDM with Hybrid Functionals: Delocalization Error and Halogen Bonding in Molecular Crystals. Journal of Chemical Theory and Computation, 2019, 15, 4933-4944.	5.3	22
28	Origin of Nanoscale Friction Contrast between Supported Graphene, MoS₂, and a Graphene/MoS₂ Heterostructure. Nano Letters, 2019, 19, 5496-5505.	9.1	115
29	PEPCONF, a diverse data set of peptide conformational energies. Scientific Data, 2019, 6, 180310.	5.3	23
30	Gold(<scp>i</scp>) sulfide: unusual bonding and an unexpected computational challenge in a simple solid. Chemical Science, 2019, 10, 6467-6475.	7.4	12
31	Pressure-induced spin transition and site-selective metallization in CoCl2. Scientific Reports, 2019, 9, 5448.	3.3	11
32	Composite and Low-Cost Approaches for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2265-2276.	5.3	18
33	Atom-Centered Potentials with Dispersion-Corrected Minimal-Basis-Set Hartreeâ€“Fock: An Efficient and Accurate Computational Approach for Large Molecular Systems. Journal of Chemical Theory and Computation, 2018, 14, 726-738.	5.3	18
34	A computational exploration of the crystal energy and charge-carrier mobility landscapes of the chiral [6]helicene molecule. Nanoscale, 2018, 10, 1865-1876.	5.6	48
35	Non-Covalent Interactions in Molecular Crystals: Exploring the Accuracy of the Exchange-Hole Dipole Moment Model with Local Orbitals. Journal of Chemical Theory and Computation, 2018, 14, 5715-5724.	5.3	9
36	Pressure-Induced Isostructural Antiferromagneticâ€“Ferromagnetic Transition in an Organic Electride. Journal of Physical Chemistry C, 2018, 122, 12742-12747.	3.1	14

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37	Quantitative Electron Delocalization in Solids from Maximally Localized Wannier Functions. Journal of Chemical Theory and Computation, 2018, 14, 4699-4710.	5.3	12
38	The effect of electronic excitation on London dispersion. Canadian Journal of Chemistry, 2018, 96, 730-737.	1.1	9
39	Transferable Atom-Centered Potentials for the Correction of Basis Set Incompleteness Errors in Density-Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 3505-3524.	5.3	29
40	Adsorption of graphene to nickel (111) using the exchange-hole dipole moment model. Carbon, 2017, 118, 184-191.	10.3	18
41	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2017, 13, 441-450.	5.3	56
42	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction II: Nonplanar Molecules. Journal of Chemical Theory and Computation, 2017, 13, 5332-5342.	5.3	31
43	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
44	Adsorption of graphene to metal (111) surfaces using the exchange-hole dipole moment model. Carbon, 2017, 124, 531-540.	10.3	22
45	Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality. ACS Nano, 2017, 11, 8329-8338.	14.6	136
46	Accurate Modeling of Water Clusters with Density-Functional Theory Using Atom-Centered Potentials. Journal of Chemical Theory and Computation, 2017, 13, 4205-4215.	5.3	10
47	Effects of the CO2 Guest Molecule on the sI Clathrate Hydrate Structure. Materials, 2016, 9, 777.	2.9	33
48	4-[(1-Benzyl-1H-1,2,3-triazol-4-yl)methoxy]benzene-1,2-dicarbonitrile: crystal structure, Hirshfeld surface analysis and energy-minimization calculations. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 563-569.	0.5	0
49	Crystallographic and computational study of t-butyl N-[3-hydroxy-1-phenyl-4-(pyridin-) Tj ETQq1 1 0.784314 rgBT /Overlo Crystalline Materials, 2016, 231, 663-672.	0.8	1
50	A conformational polymorph of Ph₃PAu[SC(OEt)=NPh] featuring an intramolecular AuÂ·Â·Â·Ï€ interaction. Zeitschrift Fur Kristallographie - Crystalline Materials, 2016, 231, 653-661.	0.8	11
51	Hydrogen bonding in 2,6-bis(4-fluorophenyl)-3,5-dimethylpiperidin-4-one methanol solvate. Zeitschrift Fur Kristallographie - Crystalline Materials, 2016, 231, 365-374.	0.8	0
52	Reevaluating the Stability and Prevalence of Conglomerates: Implications for Preferential Crystallization. Crystal Growth and Design, 2016, 16, 6055-6059.	3.0	29
53	Non-covalently generated 3D supramolecular crystal structure in a new family of hybrid nitrates templated by piperazine: Thermal behavior and in vitro antimicrobial potential. Polyhedron, 2016, 119, 238-247.	2.2	10
54	Interpretation of molecular device transport calculations. Canadian Journal of Chemistry, 2016, 94, 1022-1027.	1.1	3

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55	Evaluation of Shear-Slip Transitions in Crystalline Aspirin by Density-Functional Theory. Crystal Growth and Design, 2016, 16, 6867-6873.	3.0	17
56	Exchangeâ€“Correlation Effects for Noncovalent Interactions in Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3160-3175.	5.3	24
57	Surface Adsorption from the Exchange-Hole Dipole Moment Dispersion Model. Journal of Chemical Theory and Computation, 2016, 12, 3305-3315.	5.3	43
58	Persistence of Câ€“Hâ‹¯Ï€(chelate ring) interactions in the crystal structures of Pd(S₂COR)₂. The utility of Pd(S₂COR)₂as precursors for palladium sulphide materials. CrystEngComm, 2016, 18, 1105-1117.	2.6	26
59	Guestâ€“host interactions in gas clathrate hydrates under pressure. High Pressure Research, 2015, 35, 49-56.	1.2	9
60	Bipodal benzoylthiocarbamic acid esters: crystal and molecular structures of R = Et (a polymorph), and of a binuclear Cu(I) complex, R = iPr. Zeitschrift Fur Kristallographie - Crystalline Materials, 2015, 230, 397-405.	0.8	2
61	Chemical bonding and surface interactions in Bi2Se3 and Bi4Se3. Computational and Theoretical Chemistry, 2015, 1053, 238-244.	2.5	14
62	(Ag,Cu)â€“Taâ€“O Ternaries As High-Temperature Solid-Lubricant Coatings. ACS Applied Materials & Interfaces, 2015, 7, 15422-15429.	8.0	32
63	The importance of Auâ‹¯Ï€(aryl) interactions in the formation of spherical aggregates in binuclear phosphane gold(i) complexes of a bipodal thiocarbamate dianion: a combined crystallographic and computational study, and anti-microbial activity. RSC Advances, 2015, 5, 41401-41411.	3.6	18
64	Oscillatory motion in layered materials: graphene, boron nitride, and molybdenum disulfide. Nanotechnology, 2015, 26, 165701.	2.6	18
65	Predicting Energetics of Supramolecular Systems Using the XDM Dispersion Model. Journal of Chemical Theory and Computation, 2015, 11, 4033-4040.	5.3	39
66	Halogen Bonding from Dispersion-Corrected Density-Functional Theory: The Role of Delocalization Error. Journal of Chemical Theory and Computation, 2014, 10, 5436-5447.	5.3	100
67	Critic2: A program for real-space analysis of quantum chemical interactions in solids. Computer Physics Communications, 2014, 185, 1007-1018.	7.5	497
68	Metallophilic interactions from dispersion-corrected density-functional theory. Journal of Chemical Physics, 2014, 140, 18A504.	3.0	47
69	Unraveling Interactions in Molecular Crystals Using Dispersion Corrected Density Functional Theory: The Case of the Epoxydihydroarsanthrene Molecules. Journal of Chemical Theory and Computation, 2014, 10, 5010-5019.	5.3	6
70	Density-functional description of electrides. Physical Chemistry Chemical Physics, 2014, 16, 14584-14593.	2.8	76
71	The role of roughness-induced damping in the oscillatory motion of bilayer graphene. Nanotechnology, 2014, 25, 425703.	2.6	2
72	Modeling graphite under stress: Equations of state, vibrational modes, and interlayer friction. Physical Review B, 2014, 90, .	3.2	7

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73	Chemical Basis of the Tribological Properties of AgTaO₃ Crystal Surfaces. Journal of Physical Chemistry C, 2014, 118, 17577-17584.	3.1	18
74	Predicting the Relative Solubilities of Racemic and Enantiopure Crystals by Densityâ€Functional Theory. Angewandte Chemie - International Edition, 2014, 53, 7879-7882.	13.8	56
75	Many-body dispersion interactions from the exchange-hole dipole moment model. Journal of Chemical Physics, 2013, 138, 054103.	3.0	65
76	Performance of conventional and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. Physical Chemistry Chemical Physics, 2013, 15, 12821.	2.8	120
77	Carbon Nanotube Chirality Determines Efficiency of Electron Transfer to Fullerene in All-Carbon Photovoltaics. Journal of Physical Chemistry Letters, 2013, 4, 2914-2918.	4.6	46
78	Effect of tip shape on atomic-friction at graphite step edges. Applied Physics Letters, 2013, 103, 081601.	3.3	30
79	An empirical model for silver tantalate. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 055002.	2.0	12
80	Non-covalent interactions and thermochemistry using XDM-corrected hybrid and range-separated hybrid density functionals. Journal of Chemical Physics, 2013, 138, 204109.	3.0	130
81	Extreme density-driven delocalization error for a model solvated-electron system. Journal of Chemical Physics, 2013, 139, 184116.	3.0	93
82	Efficient basis sets for non-covalent interactions in XDM-corrected density-functional theory. Journal of Chemical Physics, 2013, 139, 214109.	3.0	29
83	Revealing non-covalent interactions in solids: NCI plots revisited. Physical Chemistry Chemical Physics, 2012, 14, 12165.	2.8	279
84	Adsorption of Organic Molecules on Kaolinite from the Exchange-Hole Dipole Moment Dispersion Model. Journal of Chemical Theory and Computation, 2012, 8, 5124-5131.	5.3	50
85	A benchmark for non-covalent interactions in solids. Journal of Chemical Physics, 2012, 137, 054103.	3.0	300
86	Van der Waals interactions in solids using the exchange-hole dipole moment model. Journal of Chemical Physics, 2012, 136, 174109.	3.0	197
87	Raman modes and GrÃ¼neisen parameters of graphite under compressive biaxial stress. Carbon, 2012, 50, 4600-4606.	10.3	28
88	Topological Partition of the Elastic Constants of Crystals. Journal of Physical Chemistry A, 2011, 115, 12953-12961.	2.5	11
89	Equations of state and thermodynamics of solids using empirical corrections in the quasiharmonic approximation. Physical Review B, 2011, 84, .	3.2	75
90	Density functional calculation for the first and second harmonic generation of the chalcopyrite Ga2AsSb. Computational Materials Science, 2011, 50, 886-892.	3.0	11

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91	Equations of state in solids: Fitting theoretical data, possibly including noise and jumps. Computational and Theoretical Chemistry, 2011, 975, 111-115.	2.5	13
92	A fast and accurate algorithm for QTAIM integration in solids. Journal of Computational Chemistry, 2011, 32, 291-305.	3.3	31
93	Gibbs2: A new version of the quasi-harmonic model code. I. Robust treatment of the static data. Computer Physics Communications, 2011, 182, 1708-1720.	7.5	299
94	Gibbs2: A new version of the quasiharmonic model code. II. Models for solid-state thermodynamics, features and implementation. Computer Physics Communications, 2011, 182, 2232-2248.	7.5	659
95	Treatment of first-principles data for predictive quasiharmonic thermodynamics of solids: The case of MgO. Physical Review B, 2011, 84, .	3.2	39
96	Supramolecular architectures based on As(lone pair)â‹¯Ï€(aryl) interactions. Chemical Communications, 2011, 47, 7608.	4.1	54
97	Ab-initio study of the structural, linear and nonlinear optical properties of CdAl2Se4 defect-chalcopyrite. Journal of Solid State Chemistry, 2010, 183, 46-51.	2.9	39
98	Elastic properties and bonding of the AgGaSe2 chalcopyrite. Physica B: Condensed Matter, 2010, 405, 3658-3664.	2.7	56
99	Topological Characterization of the Electron Density Laplacian in Crystals. The Case of the Group IV Elements. Journal of Chemical Theory and Computation, 2010, 6, 3761-3779.	5.3	42
100	Structural and thermodynamic properties of SbAsGa2 and SbPGa2 chalcopyrites. Computational Materials Science, 2010, 47, 655-659.	3.0	24
101	Critic: a new program for the topological analysis of solid-state electron densities. Computer Physics Communications, 2009, 180, 157-166.	7.5	307
102	Runwien: a text-based interface for the WIEN package. Computer Physics Communications, 2009, 180, 800-812.	7.5	22
103	First-principles study of structural, electronic, linear and nonlinear optical properties of Ga2PSb ternary chalcopyrite. European Physical Journal B, 2009, 72, 361-366.	1.5	21