Elena Arroyo-de Dompablo

List of Publications by Year
in descending order

78 papers	4,103 citations	136885 32 h-index	110317 64 g-index
81 all docs	81 docs citations	81 times ranked	4849 citing authors

#	Article	IF	Citations
1	First principles computational materials design for energy storage materials in lithium ion batteries. Energy and Environmental Science, 2009, 2, 589.	15.6	456
2	On-demand design of polyoxianionic cathode materials based on electronegativity correlations: An exploration of the Li2MSiO4 system (M=Fe, Mn, Co, Ni). Electrochemistry Communications, 2006, 8, 1292-1298.	2.3	331
3	DFT+<i>U</i> calculations of crystal lattice, electronic structure, and phase stability under pressure of TiO2 polymorphs. Journal of Chemical Physics, 2011, 135, 054503.	1.2	221
4	Achievements, Challenges, and Prospects of Calcium Batteries. Chemical Reviews, 2020, 120, 6331-6357.	23.0	219
5	Low-Potential Sodium Insertion in a NASICON-Type Structure through the Ti(III)/Ti(II) Redox Couple. Journal of the American Chemical Society, 2013, 135, 3897-3903.	6.6	213
6	On the Energetic Stability and Electrochemistry of Li₂MnSiO₄ Polymorphs. Chemistry of Materials, 2008, 20, 5574-5584.	3.2	178
7	Lattice Dynamics of Î²-V₂O₅: Raman Spectroscopic Insight into the Atomistic Structure of a High-Pressure Vanadium Pentoxide Polymorph. Inorganic Chemistry, 2012, 51, 3194-3201.	1.9	129
8	Recent Advances in First Principles Computational Research of Cathode Materials for Lithium-Ion Batteries. Accounts of Chemical Research, 2013, 46, 1171-1180.	7.6	125
9	First-principles calculations of lithium ordering and phase stability onLixNiO2. Physical Review B, 2002, 66, .	1.1	122
10	Electrochemical Intercalation of Calcium and Magnesium in TiS₂: Fundamental Studies Related to Multivalent Battery Applications. Chemistry of Materials, 2018, 30, 847-856.	3.2	105
11	Crystal Structure, Energetics, And Electrochemistry of Li₂FeSiO₄ Polymorphs from First Principles Calculations. Chemistry of Materials, 2012, 24, 495-503.	3.2	102
12	Rationalization of Intercalation Potential and Redox Mechanism for A₂Ti₃O₇ (A = Li, Na). Chemistry of Materials, 2013, 25, 4946-4956.	3.2	98
13	Improved electrode characteristics of olivineâ€“LiCoPO4 processed by high energy milling. Journal of Power Sources, 2006, 160, 523-528.	4.0	95
14	First principles investigations of complex hydrides AMH4 and A3MH6 (A=Li, Na, K, M=B, Al, Ga) as hydrogen storage systems. Journal of Alloys and Compounds, 2004, 364, 6-12.	2.8	90
15	A Joint Computational and Experimental Evaluation of CaMn₂O₄ Polymorphs as Cathode Materials for Ca Ion Batteries. Chemistry of Materials, 2016, 28, 6886-6893.	3.2	80
16	Lithium Storage Mechanisms and Effect of Partial Cobalt Substitution in Manganese Carbonate Electrodes. Inorganic Chemistry, 2012, 51, 5554-5560.	1.9	75
17	First-principles calculations on LixNiO2: phase stability and monoclinic distortion. Journal of Power Sources, 2003, 119-121, 654-657.	4.0	64
18	In quest of cathode materials for Ca ion batteries: the CaMO₃ perovskites (M = Mo, Cr,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.3	64

#	Article	IF	Citations
19	Electrochemical lithium intercalation in Li2Ti3O7-ramsdellite structure. Materials Research Bulletin, 1997, 32, 993-1001.	2.7	58
20	Synthesis and Electrochemical Properties of Layered Li0.9Ni0.45Ti0.55O2. Chemistry of Materials, 2003, 15, 4503-4507.	3.2	55
21	Assessing Si-based anodes for Ca-ion batteries: Electrochemical decalciation of CaSi2. Electrochemistry Communications, 2016, 66, 75-78.	2.3	55
22	A computational investigation on fluorinated-polyanionic compounds as positive electrode for lithium batteries. Journal of Power Sources, 2007, 174, 1251-1257.	4.0	54
23	Taking steps forward in understanding the electrochemical behavior of Na₂Ti₃O₇. Journal of Materials Chemistry A, 2015, 3, 22280-22286.	5.2	51
24	Computational Investigation of Li Insertion in Li₃VO₄. Chemistry of Materials, 2016, 28, 5643-5651.	3.2	50
25	Benefits of N for O substitution in polyoxoanionic electrode materials: a first principles investigation of the electrochemical properties of Li2FeSiO4â^’yNy (y = 0, 0.5, 1). Journal of Materials Chemistry, 2011, 21, 10026.	6.7	46
26	Computational and Experimental Investigation of the Transformation of V₂O₅ Under Pressure. Chemistry of Materials, 2007, 19, 5262-5271.	3.2	45
27	Is it possible to prepare olivine-type LiFeSiO4?A joint computational and experimental investigation. Solid State Ionics, 2008, 179, 1758-1762.	1.3	41
28	Polymorphs of Li3PO4 and Li2MSiO4 (M=Mn, Co). Journal of Power Sources, 2009, 189, 638-642.	4.0	41
29	Electrochemical Study of Li[sub 3]Fe(MoO[sub 4])[sub 3] as Positive Electrode in Lithium Cells. Journal of the Electrochemical Society, 2005, 152, A1306.	1.3	40
30	Lithium Insertion in the High-Pressure Polymorph of FePO[sub 4]. Electrochemical and Solid-State Letters, 2005, 8, A564.	2.2	40
31	High-Pressure Investigation of Li₂MnSiO₄ and Li₂CoSiO₄ Electrode Materials for Lithium-Ion Batteries. Inorganic Chemistry, 2012, 51, 5779-5786.	1.9	34
32	High pressure polymorphs of LiCoPO4 and LiCoAsO4. Solid State Sciences, 2009, 11, 343-348.	1.5	33
33	Structural Study of Electrochemically Obtained Li2+xTi3O7. Journal of Solid State Chemistry, 2000, 153, 132-139.	1.4	31
34	High pressure driven structural and electrochemical modifications in layered lithium transition metal intercalation oxides. Energy and Environmental Science, 2012, 5, 6214.	15.6	31
35	Comparative computational investigation of N and F substituted polyoxoanionic compounds. Electrochemistry Communications, 2011, 13, 1047-1050.	2.3	29
36	Comparative Investigation of MgMnSiO₄ and Olivine-Type MgMnSiS₄ as Cathode Materials for Mg Batteries. Journal of Physical Chemistry C, 2018, 122, 9356-9362.	1.5	28

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37	Analysis of Minerals as Electrode Materials for Ca-based Rechargeable Batteries. Scientific Reports, 2019, 9, 9644.	1.6	28
38	New insights into the electrochemical performance of Li₂MnSiO₄: effect of cationic substitutions. Journal of Materials Chemistry A, 2015, 3, 6004-6011.	5.2	27
39	Relation between the magnetic properties and the crystal and electronic structures of manganese spinels LiNi0.5Mn1.5O4 and LiCu0.5Mn1.5O4â^'Î´ (0<Î´<0.125). Journal of Applied Physics, 2006, 100, 093908.	1.1	26
40	First Principles Investigation of Oxygen Vacancies in Columbite MNb₂O₆ (M =) Tj ETQq0 0 0 rgBT /Overlock 1	3.2	26
41	New electrode materials for lithium rechargeable batteries. Journal of Power Sources, 1999, 81-82, 85-89.	4.0	25
42	Electrochemical Data Transferability within LiyVOXO4(X = Si, Ge0.5Si0.5, Ge, Si0.5As0.5, Si0.5P0.5, As, P) Polyoxyanionic Compounds. Chemistry of Materials, 2007, 19, 2411-2422.	3.2	24
43	An Unnoticed Inorganic Solid Electrolyte: Dilithium Sodium Phosphate with the Nalipoite Structure. Inorganic Chemistry, 2014, 53, 2310-2316.	1.9	23
44	Novel superconductors obtained by electrochemical Zn intercalation of Î²-ZrNCl and related compounds. Solid State Sciences, 2000, 2, 581-588.	0.8	22
45	Computational investigation of the influence of tetrahedral oxoanions (sulphate, selenate and) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.7	22
46	Novel olivine and spinel LiMAsO4 (M=3d-metal) as positive electrode materials in lithium cells. Solid State Ionics, 2006, 177, 2625-2628.	1.3	21
47	Are high pressure materials suitable for electrochemical applications? HP-V2O5 as a novel electrode material for Li batteries. Electrochemistry Communications, 2007, 9, 1305-1310.	2.3	21
48	Study of sodium manganese fluorides as positive electrodes for Na-ion batteries. Solid State Ionics, 2015, 278, 106-113.	1.3	21
49	DFT investigation of Ca mobility in reduced-perovskite and oxidized-marokite oxides. Energy Storage Materials, 2019, 21, 354-360.	9.5	21
50	On the Origin of the Monoclinic Distortion in LixNiO2. Chemistry of Materials, 2003, 15, 63-67.	3.2	20
51	Gaining Insights into the Energetics of FePO₄Polymorphs. Chemistry of Materials, 2010, 22, 994-1001.	3.2	20
52	Enlisting Potential Cathode Materials for Rechargeable Ca Batteries. Chemistry of Materials, 2021, 33, 2488-2497.	3.2	20
53	An Experimental and Computational Study of the Electrode Material Olivine-LiCoAsO[sub 4]. Journal of the Electrochemical Society, 2006, 153, A673.	1.3	18
54	On the Study of Ca and Mg Deintercalation from Ternary Tantalum Nitrides. ACS Omega, 2019, 4, 8943-8952.	1.6	18

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55	On the Synthesis of Ramsdellite LiTiMO4 (M = Ti, V, Cr, Mn, Fe): An Experimental and Computational Study of the Spinelâ€“Ramsdellite Transformation. European Journal of Inorganic Chemistry, 2007, 2007, 3375-3384.	1.0	17
56	Appraisal of calcium ferrites as cathodes for calcium rechargeable batteries: DFT, synthesis, characterization and electrochemistry of Ca₄Fe₉O₁₇. Dalton Transactions, 2020, 49, 2671-2679.	1.6	17
57	Structure and reaction with lithium of tetragonal pyrochlore-like compound Sm2Ti2O7. Journal of Materials Processing Technology, 1999, 92-93, 529-533.	3.1	15
58	A First-Principles Investigation of the Role Played by Oxygen Deficiency in the Electrochemical Properties of LiCu[sub 0.5]Mn[sub 1.5]O[sub 4â^'Î´] Spinels. Journal of the Electrochemical Society, 2006, 153, A2098.	1.3	15
59	Evaluation of cobalt oxides for calcium battery cathode applications. Solid State Ionics, 2019, 340, 115004.	1.3	15
60	High Pressure Effect on Structural and Electrochemical Properties of Anionic Redox-Based Lithium Transition Metal Oxides. Matter, 2021, 4, 164-181.	5.0	15
61	On the viability of Mg extraction in MgMoN₂: a combined experimental and theoretical approach. Physical Chemistry Chemical Physics, 2017, 19, 26435-26441.	1.3	11
62	Electrode characteristics of Li2Ti3O7-ramsdellite processed by mechanical grinding. Journal of Materials Science, 2002, 37, 3981-3986.	1.7	10
63	First Mixed-Metal Fluoride Pyrochlores Obtained by Topotactic Oxidation of Ammonium Fluorides under F₂ Gas. Crystal Growth and Design, 2021, 21, 935-945.	1.4	9
64	Towards innovative electrode materials obtained by high-pressure: Experimental and computational study of HP-FePO4. Journal of Physics and Chemistry of Solids, 2006, 67, 1243-1247.	1.9	8
65	A computational investigation on the electrochemical properties of spinel-like LiCoAsO4 as positive electrode for lithium-ion batteries. Solid State Sciences, 2006, 8, 916-921.	1.5	7
66	Elucidation of the redox activity of Ca2MnO3.5 and CaV2O4 in calcium batteries using operando XRD: charge compensation mechanism and reversibility. Energy Storage Materials, 2022, 47, 354-364.	9.5	7
67	A First Principles Study of Hydrogen Storage in NaAlH4-Related Complex Hydrides. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1982-1984.	0.6	6
68	Structural Evolution of Li[sub 3+x]Fe(MoO[sub 4])[sub 3] upon Lithium Insertion in the Compositional Range 0â‰xâ‰1. Journal of the Electrochemical Society, 2006, 153, A275.	1.3	6
69	Understanding sodium versus lithium intercalation potentials of electrode materials for alkali-ion batteries. Functional Materials Letters, 2014, 07, 1440003.	0.7	4
70	Synchrotron X-ray diffraction study of phase separation on heating oxidized La2CuO4.103(4): the stabilization of phase La2CuO4.086(4). Physica C: Superconductivity and Its Applications, 1999, 319, 21-33.	0.6	3
71	Electrochemical sodium insertion/extraction in Na2(MoOPO4)2(HPO4)Â·yH2O (y=2, 0). Journal of Materials Chemistry, 1998, 8, 2405-2410.	6.7	2
72	High pressure materials for energy storage: the case of V₂O₅. Journal of Physics: Conference Series, 2008, 121, 032001.	0.3	1

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73	Reactivity of Nano-LaPO4 Composites in Lithium Cells. ECS Transactions, 2010, 33, 101-110.	0.3	1
74	Combining experiments and computations to understand the intercalation potential and redox mechanism for A2Ti3O7 (A=Li, Na). Materials Research Society Symposia Proceedings, 2015, 1740, 31.	0.1	1
75	Temperature and pressure-induced strains in anhydrous iron trifluoride polymorphs. Physical Chemistry Chemical Physics, 2021, 23, 2825-2835.	1.3	1
76	Computational and Experimental investigation of Nalipoite-Li2APO4 (A = Na, K) electrolytes for Li-ion batteries. Materials Research Society Symposia Proceedings, 2015, 1740, 37.	0.1	0
77	Tackling the Development of Rechargeable Calcium Batteries: The CARBAT Project. ECS Meeting Abstracts, 2020, MA2020-02, 449-449.	0.0	0
78	Minerals As Electrode Materials for Ca-Based Rechargeable Batteries: Evaluation of the Pyroxene, Garnet, Melilite and Double Carbonate Groups. ECS Meeting Abstracts, 2020, MA2020-02, 460-460.	0.0	0