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	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
2	High Pressure Effect on Structural and Electrochemical Properties of Anionic Redox-Based Lithium Transition Metal Oxides. Matter, 2021, 4, 164-181.	5.0	15
3	Temperature and pressure-induced strains in anhydrous iron trifluoride polymorphs. Physical Chemistry Chemical Physics, 2021, 23, 2825-2835.	1.3	1
4	Enlisting Potential Cathode Materials for Rechargeable Ca Batteries. Chemistry of Materials, 2021, 33, 2488-2497.	3.2	20
5	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
6	Achievements, Challenges, and Prospects of Calcium Batteries. Chemical Reviews, 2020, 120, 6331-6357.	23.0	219
7	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
8	Tackling the Development of Rechargeable Calcium Batteries: The CARBAT Project. ECS Meeting Abstracts, 2020, MA2020-02, 449-449.	0.0	0
9	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
10	Evaluation of cobalt oxides for calcium battery cathode applications. Solid State Ionics, 2019, 340, 115004.	1.3	15
11	Analysis of Minerals as Electrode Materials for Ca-based Rechargeable Batteries. Scientific Reports, 2019, 9, 9644.	1.6	28
12	DFT investigation of Ca mobility in reduced-perovskite and oxidized-marokite oxides. Energy Storage Materials, 2019, 21, 354-360.	9.5	21
13	On the Study of Ca and Mg Deintercalation from Ternary Tantalum Nitrides. ACS Omega, 2019, 4, 8943-8952.	1.6	18
14	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
15	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
16	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
17	In quest of cathode materials for Ca ion batteries: the CaMO₃ perovskites (M = Mo, Cr,) Tj ETQq1 1 0.784314 rgBT /Overlo	1.3	64
18	Assessing Si-based anodes for Ca-ion batteries: Electrochemical decalciation of CaSi2. Electrochemistry Communications, 2016, 66, 75-78.	2.3	55

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19	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
20	Computational Investigation of Li Insertion in Li₃VO₄. Chemistry of Materials, 2016, 28, 5643-5651.	3.2	50
21	New insights into the electrochemical performance of Li₂MnSiO₄: effect of cationic substitutions. Journal of Materials Chemistry A, 2015, 3, 6004-6011.	5.2	27
22	Study of sodium manganese fluorides as positive electrodes for Na-ion batteries. Solid State Ionics, 2015, 278, 106-113.	1.3	21
23	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
24	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
25	Taking steps forward in understanding the electrochemical behavior of Na₂Ti₃O₇. Journal of Materials Chemistry A, 2015, 3, 22280-22286.	5.2	51
26	Computational investigation of the influence of tetrahedral oxoanions (sulphate, selenate and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 46	1.7	22
27	Understanding sodium versus lithium intercalation potentials of electrode materials for alkali-ion batteries. Functional Materials Letters, 2014, 07, 1440003.	0.7	4
28	An Unnoticed Inorganic Solid Electrolyte: Dilithium Sodium Phosphate with the Nalipoite Structure. Inorganic Chemistry, 2014, 53, 2310-2316.	1.9	23
29	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
30	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
31	Rationalization of Intercalation Potential and Redox Mechanism for A₂Ti₃O₇ (A = Li, Na). Chemistry of Materials, 2013, 25, 4946-4956.	3.2	98
32	High pressure driven structural and electrochemical modifications in layered lithium transition metal intercalation oxides. Energy and Environmental Science, 2012, 5, 6214.	15.6	31
33	High-Pressure Investigation of Li₂MnSiO₄ and Li₂CoSiO₄ Electrode Materials for Lithium-Ion Batteries. Inorganic Chemistry, 2012, 51, 5779-5786.	1.9	34
34	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
35	Crystal Structure, Energetics, And Electrochemistry of Li₂FeSiO₄ Polymorphs from First Principles Calculations. Chemistry of Materials, 2012, 24, 495-503.	3.2	102
36	Lithium Storage Mechanisms and Effect of Partial Cobalt Substitution in Manganese Carbonate Electrodes. Inorganic Chemistry, 2012, 51, 5554-5560.	1.9	75

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37	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
38	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
39	Comparative computational investigation of N and F substituted polyoxoanionic compounds. Electrochemistry Communications, 2011, 13, 1047-1050.	2.3	29
40	Reactivity of Nano-LaPO4 Composites in Lithium Cells. ECS Transactions, 2010, 33, 101-110.	0.3	1
41	First Principles Investigation of Oxygen Vacancies in Columbite MNb₂O₆ (M =) Tj ETQq1 1 0.784314 rgBT /O	3.2	26
42	Gaining Insights into the Energetics of FePO₄Polymorphs. Chemistry of Materials, 2010, 22, 994-1001.	3.2	20
43	High pressure polymorphs of LiCoPO4 and LiCoAsO4. Solid State Sciences, 2009, 11, 343-348.	1.5	33
44	Polymorphs of Li3PO4 and Li2MSiO4 (M=Mn, Co). Journal of Power Sources, 2009, 189, 638-642.	4.0	41
45	First principles computational materials design for energy storage materials in lithium ion batteries. Energy and Environmental Science, 2009, 2, 589.	15.6	456
46	Is it possible to prepare olivine-type LiFeSiO4?A joint computational and experimental investigation. Solid State Ionics, 2008, 179, 1758-1762.	1.3	41
47	On the Energetic Stability and Electrochemistry of Li₂MnSiO₄ Polymorphs. Chemistry of Materials, 2008, 20, 5574-5584.	3.2	178
48	High pressure materials for energy storage: the case of V₂O₅. Journal of Physics: Conference Series, 2008, 121, 032001.	0.3	1
49	Computational and Experimental Investigation of the Transformation of V₂O₅ Under Pressure. Chemistry of Materials, 2007, 19, 5262-5271.	3.2	45
50	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
51	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
52	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
53	A computational investigation on fluorinated-polyanionic compounds as positive electrode for lithium batteries. Journal of Power Sources, 2007, 174, 1251-1257.	4.0	54
54	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

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55	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
56	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
57	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
58	Improved electrode characteristics of olivineâ€"LiCoPO4 processed by high energy milling. Journal of Power Sources, 2006, 160, 523-528.	4.0	95
59	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
60	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
61	An Experimental and Computational Study of the Electrode Material Olivine-LiCoAsO[sub 4]. Journal of the Electrochemical Society, 2006, 153, A673.	1.3	18
62	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
63	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
64	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
65	Lithium Insertion in the High-Pressure Polymorph of FePO[sub 4]. Electrochemical and Solid-State Letters, 2005, 8, A564.	2.2	40
66	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
67	First-principles calculations on LixNiO2: phase stability and monoclinic distortion. Journal of Power Sources, 2003, 119-121, 654-657.	4.0	64
68	Synthesis and Electrochemical Properties of Layered Li0.9Ni0.45Ti0.55O2. Chemistry of Materials, 2003, 15, 4503-4507.	3.2	55
69	On the Origin of the Monoclinic Distortion in LixNiO2. Chemistry of Materials, 2003, 15, 63-67.	3.2	20
70	First-principles calculations of lithium ordering and phase stability onLixNiO2. Physical Review B, 2002, 66, .	1.1	122
71	Electrode characteristics of Li2Ti3O7-ramsdellite processed by mechanical grinding. Journal of Materials Science, 2002, 37, 3981-3986.	1.7	10
72	Structural Study of Electrochemically Obtained Li2+xTi3O7. Journal of Solid State Chemistry, 2000, 153, 132-139.	1.4	31

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73	Novel superconductors obtained by electrochemical Zn intercalation of Î²-ZrNCl and related compounds. Solid State Sciences, 2000, 2, 581-588.	0.8	22
74	Structure and reaction with lithium of tetragonal pyrochlore-like compound Sm2Ti2O7. Journal of Materials Processing Technology, 1999, 92-93, 529-533.	3.1	15
75	New electrode materials for lithium rechargeable batteries. Journal of Power Sources, 1999, 81-82, 85-89.	4.0	25
76	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
77	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
78	Electrochemical lithium intercalation in Li2Ti3O7-ramsdellite structure. Materials Research Bulletin, 1997, 32, 993-1001.	2.7	58