HÃ©lio Anderson Duarte

List of Publications by Year
in descending order

128 papers	4,232 citations	109321 35 h-index	128289 60 g-index
131 all docs	131 docs citations	131 times ranked	5250 citing authors

#	Article	IF	Citations
1	Arsenic adsorption on Mn3O4 surface: As(OH)3/AsO(OH)3 oxidation mechanism. Applied Surface Science, 2022, 580, 152213.	6.1	6
2	Growing Mechanism of Polysulfides and Elemental Sulfur Formation: Implications to Hindered Chalcopyrite Dissolution. Journal of Physical Chemistry A, 2022, 126, 1660-1665.	2.5	4
3	Unveiling the Zirconium and Hafnium Speciation in Fluorideâ€Nitric Acid Solutions by Paper Spray Ionization Mass Spectrometry Combined with DFT Calculations. European Journal of Inorganic Chemistry, 2021, 2021, 1175-1185.	2.0	1
4	A simple and efficient method for simultaneous quantification of levodopa and carbidopa based on controlled oxidation process. Chemical Papers, 2021, 75, 3091-3102.	2.2	2
5	Experimental and theoretical studies of the adsorption of Cu and Ni ions from wastewater by hydroxyapatite derived from eggshells. Environmental Nanotechnology, Monitoring and Management, 2021, 15, 100439.	2.9	20
6	Comparative DFT study of the oxy(hydr)oxides of iron and aluminum â€“ structural, electronic and surface properties.. Surface Science, 2021, 708, 121821.	1.9	3
7	Accurate SCC-DFTB Parametrization for Bulk Water. Journal of Chemical Theory and Computation, 2020, 16, 1768-1778.	5.3	17
8	The effect of the heteroatom (X=P, As, Si and Ge) on the geometrical and electronic properties of Î±-Keggin polyoxometalates (M=Mo, W and Nb) â€“ A DFT investigation. Journal of Molecular Structure, 2020, 1213, 128159.	3.6	12
9	Determination of an adequate bornite model for computational simulations â€“ Cu5FeS4 or Cu8Fe4S8. Journal of Molecular Structure, 2019, 1184, 72-78.	3.6	0
10	Uranium separation from acid mine drainage using anionic resins â€“ An experimental/theoretical investigation of its chemical speciation and the interaction mechanism. Journal of Environmental Chemical Engineering, 2019, 7, 102790.	6.7	11
11	Investigation on the cytotoxic effects of nitrogen-mustard-derived Schiff bases. Studies on the reactivity of the N-mustard pharmacophoric group. Journal of Molecular Structure, 2019, 1178, 274-284.	3.6	6
12	The stability and mechanism of cerium complexation with humic substances from poultry manure â€“ A combined experimental/theoretical approach. Journal of Molecular Structure, 2019, 1178, 290-297.	3.6	5
13	FERRO â€“ UM ELEMENTO QUÃMICO ESTRATÃ‰GICO QUE PERMEIA HISTÃ“RIA, ECONOMIA E SOCIEDADE. Quimica Nova, 2019, , .	0.3	3
14	Unveiling the Structural and Electronic Properties of the B-Nb₂O₅ Surfaces and Their Interaction with H₂O and H₂O₂. Journal of Physical Chemistry C, 2018, 122, 6618-6628.	3.1	18
15	Peroxoniobium inhibits leukemia cell growth. RSC Advances, 2018, 8, 10310-10313.	3.6	10
16	Adsorption of water, sulfates and chloride on arsenopyrite surface. Applied Surface Science, 2018, 434, 389-399.	6.1	20
17	Stability, Structural, and Electronic Properties of Hausmannite (Mn₃O₄) Surfaces and Their Interaction with Water. Journal of Physical Chemistry C, 2018, 122, 20841-20849.	3.1	55
18	X-ray Absorption Near-Edge Spectroscopy Calculations on Pristine and Modified Chalcopyrite Surfaces. Journal of Physical Chemistry C, 2018, 122, 20200-20209.	3.1	8

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19	Theoretical spectroscopic insights of tautomers and enantiomers of penicillamine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 184, 308-317.	3.9	5
20	Surfaces and morphologies of covellite (CuS) nanoparticles by means of ab initio atomistic thermodynamics. CrystEngComm, 2017, 19, 3078-3084.	2.6	38
21	Stability, Structure, and Electronic Properties of the Pyrite/Arsenopyrite Solidâ€“Solid Interfaceâ€“A DFT Study. Journal of Physical Chemistry C, 2017, 121, 8042-8051.	3.1	34
22	Cyclometalated ruthenium complexes from naturally occurring quinones: studies on their photophysical features, computational details and trypanocidal activity. New Journal of Chemistry, 2017, 41, 3723-3731.	2.8	12
23	Structural, Electronic, and Thermodynamic Properties of the T and B Phases of Niobia: First-Principle Calculations. Journal of Physical Chemistry A, 2017, 121, 2399-2409.	2.5	26
24	Redox Center Modification of Lapachones towards the Synthesis of Nitrogen Heterocycles as Selective Fluorescent Mitochondrial Imaging Probes. European Journal of Organic Chemistry, 2017, 2017, 3763-3773.	2.4	20
25	Polyoxomolybdate formation â€“ A thermodynamic analysis from density functional/PCM calculations. Chemical Physics Letters, 2017, 669, 104-109.	2.6	7
26	Two-dimensional crystal CuSâ€”electronic and structural properties. 2D Materials, 2017, 4, 015041.	4.4	20
27	Stability and Effects of Subsurface Oxygen in Oxide-Derived Cu Catalyst for CO₂ Reduction. Journal of Physical Chemistry C, 2017, 121, 25010-25017.	3.1	92
28	Front Cover: Redox Center Modification of Lapachones towards the Synthesis of Nitrogen Heterocycles as Selective Fluorescent Mitochondrial Imaging Probes (Eur. J. Org. Chem. 26/2017). European Journal of Organic Chemistry, 2017, 2017, 3738-3738.	2.4	0
29	Investigation on the physicochemical properties of trans -4-stilbenecarboxaldehyde-derived hydrazones and their copper(II) complexes. Polyhedron, 2017, 134, 199-206.	2.2	3
30	Oxidation Mechanism of Arsenopyrite in the Presence of Water. Journal of Physical Chemistry C, 2017, 121, 26887-26894.	3.1	14
31	DFT Study of Hydrogen-Assisted Dissociation of CO by HCO, COH, and HCOH Formation on Fe(100). Journal of Physical Chemistry C, 2016, 120, 10830-10837.	3.1	32
32	Fluorescent oxazoles from quinones for bioimaging applications. RSC Advances, 2016, 6, 76056-76063.	3.6	22
33	Molecular Simulation of Nanosized Tubular Clay Minerals. Developments in Clay Science, 2016, , 331-359.	0.5	3
34	The Stability and Structural, Electronic and Topological Properties of Covellite (001) Surfaces.. ChemistrySelect, 2016, 1, 2730-2741.	1.5	15
35	FASP: a framework for automation of Slaterâ€“Koster file parameterization. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	15
36	Methane Câ€“H bond activation by niobium oxides: Theoretical analyses of the bonding and reactivity properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>Nbo</mml:mtext></mml:mrow><mml:mi>m</mml:mi><mml (mÂ=Â1, 2; nÂ=Â0, 1, 2). Journal of Organometallic Chemistry, 2016, 802, 49-59.	1.8	9

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37	Pyrite Oxidation Mechanism by Oxygen in Aqueous Medium. Journal of Physical Chemistry C, 2016, 120, 2760-2768.	3.1	103
38	Structural, Electronic, and Mechanical Properties of Inner Surface Modified Imogolite Nanotubes. Frontiers in Materials, 2015, 2, .	2.4	12
39	Electronic and structural properties of bulk arsenopyrite and its cleavage surfaces â€“ a DFT study. RSC Advances, 2015, 5, 2013-2023.	3.6	34
40	Nanotubes with well-defined structure: imogolites. Chemical Modelling, 2015, , 151-183.	0.4	2
41	Effect of Hydrogen in Adsorption and Direct Dissociation of CO on Fe (100) Surface: A DFT Study. American Journal of Analytical Chemistry, 2015, 06, 38-46.	0.9	7
42	Benzocaine Complexation with pâ€Sulfonic Acid Calix[n]arene: Experimental (¹Hâ€NMR) and Theoretical Approaches. Chemical Biology and Drug Design, 2014, 83, 550-559.	3.2	18
43	Native Defects in Î±-Mo₂C: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 25517-25524.	3.1	20
44	Nanotubes With Well-Defined Structure: Single- and Double-Walled Imogolites. Journal of Physical Chemistry C, 2014, 118, 5945-5953.	3.1	45
45	First-Principles Calculations and Electron Density Topological Analysis of Covellite (CuS). Journal of Physical Chemistry A, 2014, 118, 5823-5831.	2.5	111
46	Structural, mechanical and electronic properties of nano-fibriform silica and its organic functionalization by dimethyl silane: a SCC-DFTB approach. Journal of Molecular Modeling, 2013, 19, 1995-2005.	1.8	5
47	Mechanism of Alcoholâ€“Water Separation in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 4124-4130.	3.1	33
48	Imogolite-like nanotubes: structure, stability, electronic and mechanical properties of the phosphorous and arsenic derivatives. Physical Chemistry Chemical Physics, 2013, 15, 4303.	2.8	25
49	Methane Dehydrogenation by Niobium Ions: A First-Principles Study of the Gas-Phase Catalytic Reactions. Organometallics, 2013, 32, 989-999.	2.3	24
50	Chemical Speciation of Metal Complexes from Chemical Shift Calculations: The Interaction of 2-Amino-N-hydroxypropanamide with V(V) in Aqueous Solution. Journal of Physical Chemistry B, 2013, 117, 11670-11680.	2.6	0
51	Chapter 6. Surface reactivity of the sulfide minerals. Chemical Modelling, 2013, , 153-182.	0.4	2
52	Reconstruction of the Chalcopyrite Surfacesâ€”A DFT Study. Journal of Physical Chemistry C, 2012, 116, 6357-6366.	3.1	94
53	Structural, Electronic, and Mechanical Properties of Single-Walled Chrysotile Nanotube Models. Journal of Physical Chemistry C, 2012, 116, 9405-9411.	3.1	37
54	As(III) immobilization on gibbsite: Investigation of the complexation mechanism by combining EXAFS analyses and DFT calculations. Geochimica Et Cosmochimica Acta, 2012, 83, 205-216.	3.9	56

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55	Combined experimental powder X-ray diffraction and DFT data to obtain the lowest energy molecular conformation of friedelin. Quimica Nova, 2012, 35, 1916-1921.	0.3	17
56	Sulfuric and hydrochloric acid adsorption on the reconstructed sulfur terminated (001) chalcopyrite surface. International Journal of Quantum Chemistry, 2012, 112, 3216-3222.	2.0	25
57	Interaction between bradykinin potentiating nonapeptide (BPP9a) and Î²-cyclodextrin: A structural and thermodynamic study. Materials Science and Engineering C, 2012, 32, 244-253.	7.3	9
58	Water Adsorption on the Reconstructed (001) Chalcopyrite Surfaces. Journal of Physical Chemistry C, 2011, 115, 10709-10717.	3.1	50
59	Stability of hydroxylamine isomers in aqueous solution: Ab initio study using continuum, cluster-continuum and Shells Theory of Solvation. Chemical Physics Letters, 2011, 518, 61-64.	2.6	15
60	Structural characteristics of chalcopyrite from a Cu(Au) ore deposit in the CarajÃ¡s Mineral Province, Brazil. Hyperfine Interactions, 2011, 203, 47-50.	0.5	0
61	DFT study of vanadyl (IV) complexes with low molecular mass ligands: Picolinate, oxalate, malonate, and maltolate. International Journal of Quantum Chemistry, 2011, 111, 1395-1402.	2.0	7
62	Structural, Electronic, and Mechanical Properties of Single-Walled Halloysite Nanotube Models. Journal of Physical Chemistry C, 2010, 114, 11358-11363.	3.1	231
63	Disulphide and metal sulphide formation on the reconstructed (0 0 1) surface of chalcopyrite: A DFT study. Applied Surface Science, 2010, 257, 1319-1324.	6.1	67
64	Selfâ€assembled Monolayers of Alkylphosphonic Acids on Aluminum Oxide Surfaces â€“ A Theoretical Study. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 1506-1512.	1.2	38
65	Molecular Dynamics of Polypeptides and Their Inclusion Compounds with Î²-Cyclodextrin in Aqueous Solution Using DCâ€“SCCâ€“DFTB/UFF Approach. Advances in Quantum Chemistry, 2010, , 145-180.	0.8	1
66	Dynamical Discrete/Continuum Linear Response Shells Theory of Solvation: Convergence Test for NH₄⁺ and OH^{â^’} Ions in Water Solution Using DFT and DFTB Methods. Journal of Physical Chemistry B, 2010, 114, 15941-15947.	2.6	20
67	Dehydrogenation of Methane by Gas-Phase Th, Th⁺, and Th²⁺: Theoretical Insights into Actinide Chemistry. Organometallics, 2010, 29, 3735-3745.	2.3	35
68	Density-functional based tight-binding: an approximate DFT method. Journal of the Brazilian Chemical Society, 2009, 20, 1193-1205.	0.6	177
69	Conformational study of 3Î²,16Î²-dihydroxyfriedelane by NMR and ab initio calculations. Structural Chemistry, 2009, 20, 1005-1011.	2.0	4
70	Platinum(II) complexes with fluoroquinolones: Synthesis and characterization of unusual metalâ€“piperazine chelates. Inorganica Chimica Acta, 2009, 362, 2060-2064.	2.4	39
71	Gas-Phase Methane Activation by the Ac+â^¹Pu+ Ions: Theoretical Insights into the Role of 5f Electrons/Orbitals in Early Actinide Chemistry. Organometallics, 2009, 28, 3203-3211.	2.3	27
72	On the nature of the interaction between H2 and metal-organic frameworks. Theoretical Chemistry Accounts, 2008, 120, 543-550.	1.4	36

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73	DFT/PCM investigation of the Mn(II) chemical speciation in aqueous solution. International Journal of Quantum Chemistry, 2008, 108, 2467-2475.	2.0	13
74	H₂ Adsorption in Metalâ€Organic Frameworks: Dispersion or Electrostatic Interactions?. Chemistry - A European Journal, 2008, 14, 6597-6600.	3.3	69
75	Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces. Surface Science, 2008, 602, 1347-1359.	1.9	97
76	Global optimization analysis of CunAum (n+m=38) clusters: Complementary ab initio calculations. Chemical Physics, 2008, 349, 91-97.	1.9	23
77	Antioxidant activity of (+)-bergeninâ€"a phytoconstituent isolated from the bark of Sacoglottis uchi Huber (Humireaceae). Organic and Biomolecular Chemistry, 2008, 6, 2713.	2.8	48
78	The iodide-catalyzed decomposition of hydrogen peroxide: mechanistic details of an old reaction as revealed by electrospray ionization mass spectrometry monitoring. Journal of the Brazilian Chemical Society, 2008, 19, 1105-1110.	0.6	14
79	Structure and Dynamics of Angiotensin (1â€7) Vasoactive Peptide in Aqueous Solution at the Densityâ€Functional Based Tightâ€Binding Level. Macromolecular Symposia, 2007, 254, 80-86.	0.7	0
80	Study of angiotensin-(1â€“7) vasoactive peptide and its Î²-cyclodextrin inclusion complexes: Complete sequence-specific NMR assignments and structural studies. Peptides, 2007, 28, 2199-2210.	2.4	104
81	Structure and Dynamics of Î²-Cyclodextrin in Aqueous Solution at the Density-Functional Tight Binding Levelâ€. Journal of Physical Chemistry A, 2007, 111, 5648-5654.	2.5	34
82	Structural and Thermodynamic Analysis of the First Mononuclear Aqueous Aluminum Citrate Complex Using DFT Calculations. Journal of Chemical Theory and Computation, 2007, 3, 930-937.	5.3	31
83	Imogolite Nanotubes: Stability, Electronic, and Mechanical Properties. ACS Nano, 2007, 1, 362-368.	14.6	172
84	Fe(II) hydrolysis in aqueous solution: A DFT study. Chemical Physics, 2007, 333, 10-17.	1.9	40
85	Raman spectroscopy and DFT calculations of As(III) complexation with a cysteine-rich biomaterial. Journal of Colloid and Interface Science, 2007, 315, 128-134.	9.4	33
86	Monte Carlo Simulation of Cisplatin Molecule in Aqueous Solution. Journal of Physical Chemistry B, 2006, 110, 12047-12054.	2.6	55
87	Density-Functional Theory Study of Iron(III) Hydrolysis in Aqueous Solution. Journal of Physical Chemistry A, 2006, 110, 7713-7718.	2.5	55
88	Synthesis and density functional calculations of the new molecule-based magnet precursor [Fe(H2opba-i)(dmso)2]Cl. Journal of the Brazilian Chemical Society, 2006, 17, 1534-1539.	0.6	6
89	An approach based on genetic algorithms and DFT for studying clusters: (H2O)n (2â©½nâ©½13) cluster analysis. Chemical Physics, 2006, 323, 553-562.	1.9	17
90	Structural model of arsenic(III) adsorbed on gibbsite based on DFT calculations. Computational and Theoretical Chemistry, 2006, 762, 17-23.	1.5	37

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91	Theoretical study of the propagation barrier of ethylene polymerization with TiR2 (R=OCH3 or CN): The importance of the Î²-agostic interactions. Computational and Theoretical Chemistry, 2006, 762, 9-15.	1.5	5
92	Spironolactone and its Complexes with Î²-cyclodextrin: Modern NMR Characterization and Structural DFTB-SCC Calculations. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2006, 56, 293-302.	1.6	12
93	DFT study of the V(IV)/V(V) oxidation mechanism in the presence of N-hydroxyacetamide. Journal of Inorganic Biochemistry, 2005, 99, 1708-1716.	3.5	8
94	Interaction of â€“CClx (x=1â€“3) with Ru2 and RuSn dimers: a density functional study. Chemical Physics, 2005, 309, 15-22.	1.9	1
95	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. ChemInform, 2005, 36, no.	0.0	0
96	DFT Ã—TB â^' a unified quantum-mechanical hybrid method. Theoretical Chemistry Accounts, 2005, 114, 68-75.	1.4	5
97	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1267-1271.	1.2	63
98	An Efficienta PosterioriTreatment for Dispersion Interaction in Density-Functional-Based Tight Binding. Journal of Chemical Theory and Computation, 2005, 1, 841-847.	5.3	275
99	Elucidation of inclusion compounds between Î²-cyclodextrin/local anaesthetics structure: a theoretical and experimental study using differential scanning calorimetry and molecular mechanics. Computational and Theoretical Chemistry, 2004, 678, 63-66.	1.5	23
100	Tunable discotic building blocks for liquid crystalline displays. Journal of Luminescence, 2004, 108, 143-147.	3.1	12
101	pKa calculation of poliprotic acid: histamine. Chemical Physics Letters, 2004, 383, 47-52.	2.6	49
102	Ab initio correlated comparative study of the torsional potentials for 2,2â€²-bipyrrole and 2,2â€²-bifuran five membered heterocyclic dimers. Chemical Physics Letters, 2003, 369, 114-124.	2.6	24
103	Density functional study of the MoxOy and MoxOy+ (x=1â€“3; y=1â€“9) oxide clusters. Chemical Physics Letters, 2003, 372, 650-658.	2.6	34
104	Chemical nature of point defects at the (VO) 2 P 2 O 7 (100) surface. Surface Science, 2003, 538, 160-170.	1.9	8
105	Potentiometric, spectrophotometric and density functional study of the interaction of -hydroxyacetamide with oxovanadium(IV): the influence of ligand to the V(IV)/V(V) oxi-reduction reaction. Journal of Inorganic Biochemistry, 2003, 95, 14-24.	3.5	13
106	Interaction of M?Sn (M?Ru, Rh, Pd) dimers with CH2 and CF2: A density functional study. International Journal of Quantum Chemistry, 2003, 95, 164-176.	2.0	7
107	Investigation of the quality of standard sulfur basis sets for molecules using a new generator coordinate method approach: Application to 2,2?-bithiophene. International Journal of Quantum Chemistry, 2003, 95, 194-204.	2.0	1
108	Propagation of flicker in electric power networks due to wind energy conversions systems. IEEE Transactions on Energy Conversion, 2002, 17, 267-272.	5.2	54

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109	Changes of local electronic structure of perfect (VO)2P2O7() surface in response to oxygen vacancy formation: effect of electron trapping. Surface Science, 2002, 513, 367-380.	1.9	15
110	Mechanism of anion retention from EXAFS and density functional calculations: arsenic (V) adsorbed on gibbsite. Geochimica Et Cosmochimica Acta, 2001, 65, 1211-1217.	3.9	187
111	Density functional study of the first-row transition-metal complexes Mâ€“CH2, Mâ€“CHF, and Mâ€“CF2. Journal of Chemical Physics, 2001, 115, 1747-1756.	3.0	15
112	Ãndices de reatividade quÃmica a partir da teoria do funcional de densidade: formalismo e perspectivas. Quimica Nova, 2001, 24, 501-508.	0.3	6
113	Quantum-mechanical study of the interaction of Î±-cyclodextrin with methyl mercury chloride. Chemical Physics Letters, 2000, 319, 569-575.	2.6	41
114	Energy Gaps of Î±,Î±â€˜-Substituted Oligothiophenes from Semiempirical, Ab Initio, and Density Functional Methods. Journal of Physical Chemistry A, 2000, 104, 8256-8262.	2.5	114
115	Improved quantum mechanical study of the potential energy surface for the bithiophene molecule. Journal of Chemical Physics, 2000, 113, 4206-4215.	3.0	61
116	Binary Ironâ“Dinitrogen Compounds Synthesized by Co-deposition of Mass-Selected Fe, Fe2, and Fe3with N2. Journal of the American Chemical Society, 2000, 122, 6039-6044.	13.7	15
117	A physicochemical study of the tetracycline coordination to oxovanadium(IV). Journal of Inorganic Biochemistry, 1999, 76, 221-230.	3.5	26
118	Importance of Tautomers in the Chemical Behavior of Tetracyclinesâ€. Journal of Pharmaceutical Sciences, 1999, 88, 111-120.	3.3	105
119	NO adsorption on Pd clusters. A density functional study. Topics in Catalysis, 1999, 9, 123-133.	2.8	17
120	Fe(N2)n(n= 1â“5):Â Structure, Bonding, and Vibrations from Density Functional Theory. Inorganic Chemistry, 1999, 38, 3895-3903.	4.0	29
121	Interaction of N-hydroxyacetamide with vanadate: A density functional study. Journal of Inorganic Biochemistry, 1998, 72, 71-77.	3.5	23
122	Density functional study of the NO dimer using GGA and LAP functionals. Journal of Chemical Physics, 1998, 109, 26-35.	3.0	47
123	Embedded cluster model for chemisorption using density functional calculations: Oxygen adsorption on the Al(100) surface.. Journal of Chemical Physics, 1998, 108, 743-756.	3.0	29
124	Density functional study of mononitrosyls of first-row transition-metal atoms. Journal of Chemical Physics, 1997, 106, 8778-8787.	3.0	45
125	NO/Ni, NO/Ni2, and (NO)2/Ni2Interactions. A Density Functional Study. Journal of Physical Chemistry B, 1997, 101, 7464-7471.	2.6	16
126	Clay Mineral Nanotubes: Stability, Structure and Properties. , 0, , .		4

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127	Modeling the oxidation mechanism of pyrite and arsenopyrite â€“ connection to acid rock drainage. Chemical Modelling, 0, , 162-194.	0.4	0
128	The Oxidation Mechanism of Pyrites and the Sustainable Exploration of the Mineral Resources â€“ The Computational Chemistry Contribution. Revista Virtual De Quimica, 0, , .	0.4	0