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	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
2	Structural, Electronic, and Mechanical Properties of Single-Walled Halloysite Nanotube Models. Journal of Physical Chemistry C, 2010, 114, 11358-11363.	3.1	231
3	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
4	Density-functional based tight-binding: an approximate DFT method. Journal of the Brazilian Chemical Society, 2009, 20, 1193-1205.	0.6	177
5	Imogolite Nanotubes: Stability, Electronic, and Mechanical Properties. ACS Nano, 2007, 1, 362-368.	14.6	172
6	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
7	First-Principles Calculations and Electron Density Topological Analysis of Covellite (CuS). Journal of Physical Chemistry A, 2014, 118, 5823-5831.	2.5	111
8	Importance of Tautomers in the Chemical Behavior of Tetracyclinesâ€. Journal of Pharmaceutical Sciences, 1999, 88, 111-120.	3.3	105
9	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
10	Pyrite Oxidation Mechanism by Oxygen in Aqueous Medium. Journal of Physical Chemistry C, 2016, 120, 2760-2768.	3.1	103
11	Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces. Surface Science, 2008, 602, 1347-1359.	1.9	97
12	Reconstruction of the Chalcopyrite Surfacesâ€”A DFT Study. Journal of Physical Chemistry C, 2012, 116, 6357-6366.	3.1	94
13	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
14	H₂ Adsorption in Metalâ€Organic Frameworks: Dispersion or Electrostatic Interactions?. Chemistry - A European Journal, 2008, 14, 6597-6600.	3.3	69
15	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
16	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1267-1271.	1.2	63
17	Improved quantum mechanical study of the potential energy surface for the bithiophene molecule. Journal of Chemical Physics, 2000, 113, 4206-4215.	3.0	61
18	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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19	Monte Carlo Simulation of Cisplatin Molecule in Aqueous Solution. Journal of Physical Chemistry B, 2006, 110, 12047-12054.	2.6	55
20	Density-Functional Theory Study of Iron(III) Hydrolysis in Aqueous Solution. Journal of Physical Chemistry A, 2006, 110, 7713-7718.	2.5	55
21	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
22	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
23	Water Adsorption on the Reconstructed (001) Chalcopyrite Surfaces. Journal of Physical Chemistry C, 2011, 115, 10709-10717.	3.1	50
24	pKa calculation of poliprotic acid: histamine. Chemical Physics Letters, 2004, 383, 47-52.	2.6	49
25	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
26	Density functional study of the NO dimer using GGA and LAP functionals. Journal of Chemical Physics, 1998, 109, 26-35.	3.0	47
27	Density functional study of mononitrosyls of first-row transition-metal atoms. Journal of Chemical Physics, 1997, 106, 8778-8787.	3.0	45
28	Nanotubes With Well-Defined Structure: Single- and Double-Walled Imogolites. Journal of Physical Chemistry C, 2014, 118, 5945-5953.	3.1	45
29	Quantum-mechanical study of the interaction of Î±-cyclodextrin with methyl mercury chloride. Chemical Physics Letters, 2000, 319, 569-575.	2.6	41
30	Fe(II) hydrolysis in aqueous solution: A DFT study. Chemical Physics, 2007, 333, 10-17.	1.9	40
31	Platinum(II) complexes with fluoroquinolones: Synthesis and characterization of unusual metalâ€"piperazine chelates. Inorganica Chimica Acta, 2009, 362, 2060-2064.	2.4	39
32	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
33	Surfaces and morphologies of covellite (CuS) nanoparticles by means of ab initio atomistic thermodynamics. CrystEngComm, 2017, 19, 3078-3084.	2.6	38
34	Structural model of arsenic(III) adsorbed on gibbsite based on DFT calculations. Computational and Theoretical Chemistry, 2006, 762, 17-23.	1.5	37
35	Structural, Electronic, and Mechanical Properties of Single-Walled Chrysotile Nanotube Models. Journal of Physical Chemistry C, 2012, 116, 9405-9411.	3.1	37
36	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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37	Dehydrogenation of Methane by Gas-Phase Th, Th⁺, and Th²⁺: Theoretical Insights into Actinide Chemistry. Organometallics, 2010, 29, 3735-3745.	2.3	35
38	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
39	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
40	Electronic and structural properties of bulk arsenopyrite and its cleavage surfaces â€“ a DFT study. RSC Advances, 2015, 5, 2013-2023.	3.6	34
41	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
42	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
43	Mechanism of Alcoholâ€“Water Separation in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 4124-4130.	3.1	33
44	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
45	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
46	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
47	Fe(N2)n(n= 1â^'5):Â Structure, Bonding, and Vibrations from Density Functional Theory. Inorganic Chemistry, 1999, 38, 3895-3903.	4.0	29
48	Gas-Phase Methane Activation by the Ac+â^'Pu+ Ions: Theoretical Insights into the Role of 5f Electrons/Orbitals in Early Actinide Chemistry. Organometallics, 2009, 28, 3203-3211.	2.3	27
49	A physicochemical study of the tetracycline coordination to oxovanadium(IV). Journal of Inorganic Biochemistry, 1999, 76, 221-230.	3.5	26
50	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
51	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
52	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
53	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
54	Methane Dehydrogenation by Niobium Ions: A First-Principles Study of the Gas-Phase Catalytic Reactions. Organometallics, 2013, 32, 989-999.	2.3	24

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55	Interaction of N-hydroxyacetamide with vanadate: A density functional study. Journal of Inorganic Biochemistry, 1998, 72, 71-77.	3.5	23
56	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
57	Global optimization analysis of CunAum (n+m=38) clusters: Complementary ab initio calculations. Chemical Physics, 2008, 349, 91-97.	1.9	23
58	Fluorescent oxazoles from quinones for bioimaging applications. RSC Advances, 2016, 6, 76056-76063.	3.6	22
59	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
60	Native Defects in Î±-Mo₂C: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 25517-25524.	3.1	20
61	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
62	Two-dimensional crystal CuSâ€”electronic and structural properties. 2D Materials, 2017, 4, 015041.	4.4	20
63	Adsorption of water, sulfates and chloride on arsenopyrite surface. Applied Surface Science, 2018, 434, 389-399.	6.1	20
64	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
65	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
66	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
67	NO adsorption on Pd clusters. A density functional study. Topics in Catalysis, 1999, 9, 123-133.	2.8	17
68	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
69	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
70	Accurate SCC-DFTB Parametrization for Bulk Water. Journal of Chemical Theory and Computation, 2020, 16, 1768-1778.	5.3	17
71	NO/Ni, NO/Ni2, and (NO)2/Ni2Interactions. A Density Functional Study. Journal of Physical Chemistry B, 1997, 101, 7464-7471.	2.6	16
72	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

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73	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
74	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
75	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
76	The Stability and Structural, Electronic and Topological Properties of Covellite (001) Surfaces.. ChemistrySelect, 2016, 1, 2730-2741.	1.5	15
77	FASP: a framework for automation of Slaterâ€“Koster file parameterization. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	15
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	Oxidation Mechanism of Arsenopyrite in the Presence of Water. Journal of Physical Chemistry C, 2017, 121, 26887-26894.	3.1	14
80	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
81	DFT/PCM investigation of the Mn(II) chemical speciation in aqueous solution. International Journal of Quantum Chemistry, 2008, 108, 2467-2475.	2.0	13
82	Tunable discotic building blocks for liquid crystalline displays. Journal of Luminescence, 2004, 108, 143-147.	3.1	12
83	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
84	Structural, Electronic, and Mechanical Properties of Inner Surface Modified Imogolite Nanotubes. Frontiers in Materials, 2015, 2, .	2.4	12
85	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
86	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
87	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
88	Peroxoniobium inhibits leukemia cell growth. RSC Advances, 2018, 8, 10310-10313.	3.6	10
89	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
90	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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91	Chemical nature of point defects at the (VO) 2 P 2 O 7 (100) surface. Surface Science, 2003, 538, 160-170.	1.9	8
92	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
93	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
94	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
95	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
96	Polyoxomolybdate formation â€“ A thermodynamic analysis from density functional/PCM calculations. Chemical Physics Letters, 2017, 669, 104-109.	2.6	7
97	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
98	Ãndices de reatividade quÃmica a partir da teoria do funcional de densidade: formalismo e perspectivas. Quimica Nova, 2001, 24, 501-508.	0.3	6
99	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
100	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
101	Arsenic adsorption on Mn3O4 surface: As(OH)3/AsO(OH)3 oxidation mechanism. Applied Surface Science, 2022, 580, 152213.	6.1	6
102	DFT Ã—TB â^' a unified quantum-mechanical hybrid method. Theoretical Chemistry Accounts, 2005, 114, 68-75.	1.4	5
103	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
104	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
105	Theoretical spectroscopic insights of tautomers and enantiomers of penicillamine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 184, 308-317.	3.9	5
106	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
107	Conformational study of 3Î²,16Î²-dihydroxyfriedelane by NMR and ab initio calculations. Structural Chemistry, 2009, 20, 1005-1011.	2.0	4
108	Clay Mineral Nanotubes: Stability, Structure and Properties. , 0, , .		4

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109	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
110	Molecular Simulation of Nanosized Tubular Clay Minerals. Developments in Clay Science, 2016, , 331-359.	0.5	3
111	Investigation on the physicochemical properties of trans -4-stilbenecarboxaldehyde-derived hydrazones and their copper(II) complexes. Polyhedron, 2017, 134, 199-206.	2.2	3
112	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
113	FERRO â€“ UM ELEMENTO QUÃMICO ESTRATÃ‰GICO QUE PERMEIA HISTÃ“RIA, ECONOMIA E SOCIEDADE. Quimica Nova, 2019, , .	0.3	3
114	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
115	Nanotubes with well-defined structure: imogolites. Chemical Modelling, 2015, , 151-183.	0.4	2
116	Chapter 6. Surface reactivity of the sulfide minerals. Chemical Modelling, 2013, , 153-182.	0.4	2
117	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
118	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
119	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
120	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
121	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. ChemInform, 2005, 36, no.	0.0	0
122	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
123	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
124	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
125	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
126	Determination of an adequate bornite model for computational simulations â€“ Cu5FeS4 or Cu8Fe4S8. Journal of Molecular Structure, 2019, 1184, 72-78.	3.6	0

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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