Alfonso HernÃ¡ndez-Laguna

List of Publications by Year
in descending order

64 papers	1,258 citations	304743 22 h-index	395702 33 g-index
65 all docs	65 docs citations	65 times ranked	972 citing authors

#	Article	IF	Citations
1	Melatonin/nanoclay hybrids for skin delivery. Applied Clay Science, 2022, 218, 106417.	5.2	2
2	Effects of the cation ordering in Mg:Al and Zn:Al layered double hydroxides on crystallographic and spectroscopical properties by means of first principles calculations. Applied Clay Science, 2022, 223, 106496.	5.2	6
3	DFT study of electronic and redox properties of TiO2 supported on olivine for modelling regolith on Moon and Mars conditions. Planetary and Space Science, 2020, 180, 104760.	1.7	4
4	DFT study of the reduction reaction of calcium perchlorate on olivine surface: Implications to formation of Martianâ€™s regolith. Applied Surface Science, 2020, 512, 145634.	6.1	5
5	Theoretical study of the gas-phase thermolysis reaction of 3,6-dimethyl-1,2,4,5-tetroxane. Methyl and axial-equatorial substitution effects. Journal of Molecular Modeling, 2019, 25, 217.	1.8	0
6	Compressibility of 2M1 muscovite-phlogopite series minerals. Journal of Molecular Modeling, 2019, 25, 341.	1.8	1
7	A DFT study of the adsorption of glycine in the interlayer space of montmorillonite. Physical Chemistry Chemical Physics, 2017, 19, 14961-14971.	2.8	28
8	Simulating the Dehydroxylation Reaction in Smectite Models by Carâ€“Parrinello-likeâ€“Bornâ€“Oppenheimer Molecular Dynamics and Metadynamics. Journal of Physical Chemistry C, 2016, 120, 28186-28192.	3.1	4
9	Compressibility of 2M₁muscovite-paragonite series minerals: A computational study to 6 GPa. American Mineralogist, 2016, 101, 1207-1216.	1.9	3
10	Hydrolysis reaction of 2,4-dichlorophenoxyacetic acid. A kinetic and computational study. Chemical Physics Letters, 2015, 639, 57-62.	2.6	4
11	Computer simulations of cations orderâ€disorder in 2:1 dioctahedral phyllosilicates using cationâ€exchange potentials and monte carlo methods. International Journal of Quantum Chemistry, 2014, 114, 1257-1286.	2.0	10
12	Theoretical study on the influence of the Mg2+ and Al3+ octahedral cations on the vibrational spectra of the hydroxy groups of dioctahedral 2:1 phyllosilicate models. Journal of Molecular Modeling, 2014, 20, 2402.	1.8	4
13	DFT study of the mechanism of the reaction of aminoguanidine with methylglyoxal. Journal of Molecular Modeling, 2014, 20, 2202.	1.8	12
14	Theoretical study of the gas-phase thermolysis of 3-methyl-1,2,4,5-tetroxane. Journal of Molecular Modeling, 2014, 20, 2224.	1.8	1
15	Theoretical study of the hydrogen bonding and infrared spectroscopy in the cis-vacant polymorph of dioctahedral 2:1 phyllosilicates. Journal of Molecular Modeling, 2014, 20, 2404.	1.8	9
16	Adsorption of Molecules onto (101Ì…4) Dolomite Surface: An Application of Computational Studies for Microcalorimetry. Journal of Physical Chemistry C, 2013, 117, 17583-17590.	3.1	26
17	Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum Mechanical Simulations. Journal of Physical Chemistry C, 2013, 117, 7526-7532.	3.1	7
18	A Tuned LRC-DFT Design of Ambipolar Diketopyrrolopyrrole-Containing Quinoidal Molecules Interesting for Molecular Electronics. Journal of Chemical Theory and Computation, 2013, 9, 2591-2601.	5.3	10

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19	A DFT Study of the Amadori Rearrangement above a Phosphatidylethanolamine Surface: Comparison to Reactions in Aqueous Environment. Journal of Physical Chemistry C, 2013, 117, 8299-8309.	3.1	10
20	Cation arrangement in the octahedral and tetrahedral sheets of cis-vacant polymorph of dioctahedral 2:1 phyllosilicates by quantum mechanical calculations. American Mineralogist, 2013, 98, 724-735.	1.9	10
21	Computational study of the elastic behavior of the 2M1 muscovite-paragonite series. American Mineralogist, 2013, 98, 651-664.	1.9	12
22	Ab Initio Molecular Dynamics Study of the Dehydroxylation Reaction in a Smectite Model. Journal of Physical Chemistry C, 2012, 116, 12203-12211.	3.1	14
23	DFT study of the adsorption of Ni on Anatase (001) surface. Computational and Theoretical Chemistry, 2012, 981, 59-67.	2.5	21
24	A comparative DFT study of the Schiff base formation from acetaldehyde and butylamine, glycine and phosphatidylethanolamine. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	13
25	Gas-phase thermolysis reaction of formaldehyde diperoxide. Kinetic study and theoretical mechanisms. Chemical Physics, 2012, 393, 37-45.	1.9	5
26	Influence of the alkyl and alkoxy side chains on the electronic structure and charge-transport properties of polythiophene derivatives. Physical Chemistry Chemical Physics, 2011, 13, 10091.	2.8	10
27	Influence of the exchangeable cation on the adsorption of 2-nitro-1-propanol on smectite surface models. Chemical Physics Letters, 2011, 515, 49-55.	2.6	3
28	Vibrations of H+(D+) in stoichiometric LiNbO3 single crystal. Journal of Chemical Physics, 2011, 135, 124501.	3.0	9
29	Structure of OH^{â^'}defects in LiNbO₃. IOP Conference Series: Materials Science and Engineering, 2010, 15, 012015.	0.6	11
30	DFT approach to reaction mechanisms through molecular complexes. The case of an organo-catalysed nucleosidation reaction. Computational and Theoretical Chemistry, 2010, 944, 43-52.	1.5	4
31	High-pressure behavior of 2M1 muscovite. American Mineralogist, 2010, 95, 249-259.	1.9	18
32	Exploring the Rehydroxylation Reaction of Pyrophyllite by Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 7593-7601.	2.6	17
33	Density functional theory and Monte Carlo study of octahedral cation ordering of Al/Fe/Mg cations in dioctahedral 2:1 phyllosilicates. American Mineralogist, 2010, 95, 209-220.	1.9	32
34	Theoretical study of the adsorption of 2-nitro-1-propanol on smectite surface models. Computational and Theoretical Chemistry, 2009, 912, 95-104.	1.5	9
35	Crystal structure and hydroxyl group vibrational frequencies of phyllosilicates by DFT methods. Computational and Theoretical Chemistry, 2009, 912, 82-87.	1.5	24
36	Dehydroxylation mechanisms in Al3+/Fe3+ dioctahedral phyllosilicates by quantum mechanical methods with cluster models. Geochimica Et Cosmochimica Acta, 2008, 72, 3929-3938.	3.9	31

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37	DFT Research on the Dehydroxylation Reaction of Pyrophyllite 2. Characterization of Reactants, Intermediates, And Transition States along the Reaction Path. Journal of Physical Chemistry A, 2008, 112, 6373-6383.	2.5	17
38	Quantum Chemistry and Computational Kinetics of the Reaction between OH Radicals and Formaldehyde Adsorbed on Small Silica Aerosol Models. Journal of Physical Chemistry C, 2008, 112, 4590-4600.	3.1	19
39	DFT Research on the Dehydroxylation Reaction of Pyrophyllite 1. First-Principle Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 7051-7060.	2.6	43
40	DFT calculation of crystallographic properties of dioctahedral 2:1 phyllosilicates. Clay Minerals, 2008, 43, 351-361.	0.6	38
41	Soft Coulomb hole method applied to molecules. International Journal of Quantum Chemistry, 2007, 107, 1046-1059.	2.0	0
42	DFT study of the cation arrangements in the octahedral and tetrahedral sheets of dioctahedral 2:1 phyllosilicates. Physics and Chemistry of Minerals, 2006, 33, 655-666.	0.8	45
43	DFT critical points of the internal rotation potential energy surface and infrared spectra of the [1H], [2H] 2,5-pyrazinedicarboxamide. Computational and Theoretical Chemistry, 2005, 714, 73-79.	1.5	2
44	Quantum mechanical calculations of trans-vacant and cis-vacant polymorphism in dioctahedral 2:1 phyllosilicates. American Mineralogist, 2005, 90, 1827-1834.	1.9	35
45	Effect of the Tetrahedral Charge on the Order-disorder of the Cation Distribution in the Octahedral Sheet of Smectites and Illites by Computational Methods. Clays and Clay Minerals, 2004, 52, 357-374.	1.3	12
46	Pyrophyllite dehydroxylation process by First Principles calculations. American Mineralogist, 2004, 89, 1092-1100.	1.9	31
47	A computational investigation of the Al/Fe/Mg order-disorder behavior in the dioctahedral sheet of phyllosilicates. American Mineralogist, 2004, 89, 164-175.	1.9	30
48	Octahedral cation ordering of illite and smectite. Theoretical exchange potential determination and Monte Carlo simulations. Physics and Chemistry of Minerals, 2003, 30, 382-392.	0.8	33
49	Isomorphous cation substitution in dioctahedral phyllosilicates by means of ab initio quantum mechanical calculations on clusters. American Mineralogist, 2003, 88, 1788-1795.	1.9	29
50	Monte Carlo simulations of ordering of Al, Fe, and Mg cations in the octahedral sheet of smectites and illites. American Mineralogist, 2003, 88, 1033-1045.	1.9	46
51	Quantum mechanical calculations of dioctahedral 2:1 phyllosilicates: Effect of octahedral cation distributions in pyrophyllite, illite, and smectite. American Mineralogist, 2002, 87, 958-965.	1.9	73
52	Isomeric adduct stability in the addition of atomic radicals to toluene: H, O(3P), F and Cl. Physical Chemistry Chemical Physics, 2002, 4, 5730-5738.	2.8	9
53	Modeling of dioctahedral 2:1 phyllosilicates by means of transferable empirical potentials. Physics and Chemistry of Minerals, 2001, 28, 130-141.	0.8	78
54	Theoretical modelling of cis â€Š-vacant and trans â€Š-vacant configurations in the octahedral sheet of illites and smectites. Physics and Chemistry of Minerals, 2001, 28, 322-331.	0.8	39

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55	Isomorphous substitution effect on the vibration frequencies of hydroxyl groups in molecular cluster models of the clay octahedral sheet. American Mineralogist, 2000, 85, 1038-1045.	1.9	50
56	Adsorption Mechanism and Structure of the Montmorillonite Complexes with (CH3)2XO (X=C, and S), (CH3O)3PO, and CH3â€“CN Molecules. Journal of Colloid and Interface Science, 2000, 222, 125-136.	9.4	20
57	Reaction mechanism of the acyl-enzyme formation in Î²-lactam hydrolysis by means of quantum chemical modeling. Computational and Theoretical Chemistry, 2000, 504, 13-28.	1.5	11
58	New Channels in the Reaction Mechanism of the Atmospheric Oxidation of Toluene. Journal of Physical Chemistry A, 2000, 104, 7847-7855.	2.5	71
59	trans-2,2â€²-Dinitrostilbene as a precursor of o-nitrobenzaldehyde, a key intermediate for pharmaceuticals: reactivity and molecular structure studies. Journal of the Chemical Society Perkin Transactions II, 1999, , 1489-1496.	0.9	5
60	Quantum mechanical and QSAR study of some Î±-arylpropionic acids as anti-inflammatory agents. European Journal of Medicinal Chemistry, 1998, 33, 103-112.	5.5	27
61	Vibrational spectrum of pyrazinecarbaldehyde. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 43-48.	1.7	4
62	Quantum Mechanical Study and Nuclear Magnetic Resonance Measurements of Some Î±-Arylcarboxyalkyl Acids as Anti-inflammatory Agents. Journal of Pharmaceutical Sciences, 1989, 78, 764-766.	3.3	6
63	Self-Consistent Fieldâ€“Molecular Orbital (SCFâ€“MO) Calculations and Nuclear Magnetic Resonance Measurements for Fosfomycin and Related Compounds. Journal of Pharmaceutical Sciences, 1987, 76, 753-756.	3.3	25
64	Quantum Mechanical Calculations Useful For Determining the Mechanism of Action of Fosfomycin. Journal of Pharmaceutical Sciences, 1983, 72, 1011-1014.	3.3	13