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	Modeling of dioctahedral 2:1 phyllosilicates by means of transferable empirical potentials. Physics and Chemistry of Minerals, 2001, 28, 130-141.	0.8	78
2	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
3	New Channels in the Reaction Mechanism of the Atmospheric Oxidation of Toluene. Journal of Physical Chemistry A, 2000, 104, 7847-7855.	2.5	71
4	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
5	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
6	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
7	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
8	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
9	DFT calculation of crystallographic properties of dioctahedral 2:1 phyllosilicates. Clay Minerals, 2008, 43, 351-361.	0.6	38
10	Quantum mechanical calculations of trans-vacant and cis-vacant polymorphism in dioctahedral 2:1 phyllosilicates. American Mineralogist, 2005, 90, 1827-1834.	1.9	35
11	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
12	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
13	Pyrophyllite dehydroxylation process by First Principles calculations. American Mineralogist, 2004, 89, 1092-1100.	1.9	31
14	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
15	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
16	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
17	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
18	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

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19	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
20	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
21	Crystal structure and hydroxyl group vibrational frequencies of phyllosilicates by DFT methods. Computational and Theoretical Chemistry, 2009, 912, 82-87.	1.5	24
22	DFT study of the adsorption of Ni on Anatase (001) surface. Computational and Theoretical Chemistry, 2012, 981, 59-67.	2.5	21
23	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
24	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
25	High-pressure behavior of 2M1 muscovite. American Mineralogist, 2010, 95, 249-259.	1.9	18
26	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
27	Exploring the Rehydroxylation Reaction of Pyrophyllite by Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 7593-7601.	2.6	17
28	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
29	Quantum Mechanical Calculations Useful For Determining the Mechanism of Action of Fosfomycin. Journal of Pharmaceutical Sciences, 1983, 72, 1011-1014.	3.3	13
30	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
31	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
32	Computational study of the elastic behavior of the 2M1 muscovite-paragonite series. American Mineralogist, 2013, 98, 651-664.	1.9	12
33	DFT study of the mechanism of the reaction of aminoguanidine with methylglyoxal. Journal of Molecular Modeling, 2014, 20, 2202.	1.8	12
34	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
35	Structure of OH^{â^’}defects in LiNbO₃. IOP Conference Series: Materials Science and Engineering, 2010, 15, 012015.	0.6	11
36	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

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37	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
38	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
39	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
40	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
41	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
42	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
43	Vibrations of H+(D+) in stoichiometric LiNbO3 single crystal. Journal of Chemical Physics, 2011, 135, 124501.	3.0	9
44	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
45	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
46	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
47	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
48	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
49	Gas-phase thermolysis reaction of formaldehyde diperoxide. Kinetic study and theoretical mechanisms. Chemical Physics, 2012, 393, 37-45.	1.9	5
50	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
51	Vibrational spectrum of pyrazinecarbaldehyde. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 43-48.	1.7	4
52	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
53	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
54	Hydrolysis reaction of 2,4-dichlorophenoxyacetic acid. A kinetic and computational study. Chemical Physics Letters, 2015, 639, 57-62.	2.6	4

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55	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
56	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
57	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
58	Compressibility of 2M₁muscovite-paragonite series minerals: A computational study to 6 GPa. American Mineralogist, 2016, 101, 1207-1216.	1.9	3
59	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
60	Melatonin/nanoclay hybrids for skin delivery. Applied Clay Science, 2022, 218, 106417.	5.2	2
61	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
62	Compressibility of 2M1 muscovite-phlogopite series minerals. Journal of Molecular Modeling, 2019, 25, 341.	1.8	1
63	Soft Coulomb hole method applied to molecules. International Journal of Quantum Chemistry, 2007, 107, 1046-1059.	2.0	0
64	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