Fernando MS Silva Fernandes

List of Publications by Year
in descending order

40	377	759233 12	839539 18
papers	citations	h-index	g-index

45	45	45	397
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Progress in the understanding of tyramine electropolymerisation mechanism. Journal of Solid State Electrochemistry, 2007, 11, 1059-1069.	2.5	36
2	Ab initio study of the conformational equilibrium of ethylene glycol. Theoretica Chimica Acta, 1991, 78, 271-280.	0.8	33
3	Phase diagrams of alkali halides using two interaction models: A molecular dynamics and free energy study. Journal of Chemical Physics, 2007, 126, 024503.	3.0	21
4	A force field for simulating ethanol adsorption on Au(111) surfaces. A DFT study. International Journal of Quantum Chemistry, 2007, 107, 2169-2177.	2.0	20
5	Modelling water adsorption on Au(210) surfaces. I. A force field for waterâ€“Au interactions by DFT. Journal of Electroanalytical Chemistry, 2007, 609, 140-146.	3.8	20
6	Mapping Potential Energy Surfaces by Neural Networks: The ethanol/Au(111) interface. Journal of Electroanalytical Chemistry, 2008, 624, 109-120.	3.8	20
7	Monte Carlo Simulation of the Phase Diagram of C60Using Two Interaction Potentials. Enthalpies of Sublimation. Journal of Physical Chemistry B, 2002, 106, 10227-10232.	2.6	19
8	Vapor-Liquid Equilibrium and Structure of Methyl Iodide Liquid. The Journal of Physical Chemistry, 1995, 99, 5180-5186.	2.9	18
9	Molecular dynamics of phase transitions in clusters of alkali halides. International Journal of Quantum Chemistry, 2001, 84, 169-180.	2.0	18
10	Modelling water adsorption on Au(210) surfaces: II. Monte Carlo simulations. Journal of Electroanalytical Chemistry, 2008, 612, 179-185.	3.8	14
11	Neural networks to approach potential energy surfaces: Application to a molecular dynamics simulation. International Journal of Quantum Chemistry, 2007, 107, 2120-2132.	2.0	13
12	A study of 1-decanethiol self-assembly on gold electrodes by computer simulation. Journal of Electroanalytical Chemistry, 2005, 574, 321-331.	3.8	12
13	A Monte Carlo and transfer-matrix grid path-integral study of the vibrational structure of Br2 in solid argon. Chemical Physics Letters, 1991, 184, 53-60.	2.6	10
14	Phase Diagrams and Sublimation Enthalpies of Model Cnâ©¾60Fullerenes:Â A Comparative Study by Computer Simulation. Journal of Physical Chemistry B, 2003, 107, 276-281.	2.6	10
15	Phase Diagram and Sublimation Enthalpies of Model C60Revisited. Journal of Physical Chemistry B, 2004, 108, 9251-9255.	2.6	10
16	Melting, freezing and nucleation in nanoclusters of potassium chloride. European Physical Journal D, 2006, 40, 115-123.	1.3	10
17	Approach to potential energy surfaces by neural networks. A review of recent work. International Journal of Quantum Chemistry, 2010, 110, 432-445.	2.0	10
18	Vapor-Liquid Equilibrium of Argon. Simulation with Nonadditive Potentials. The Journal of Physical Chemistry, 1994, 98, 3917-3920.	2.9	9

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19	The starting state in simulations of the fluidâ€“solid coexistence by Gibbsâ€“Duhem integration. Computer Physics Communications, 2001, 141, 403-411.	7.5	8
20	Melting, freezing and nucleation in nanoclusters of potassium chloride. European Physical Journal D, 2007, 41, 113-119.	1.3	8
21	Hypervolumes in microcanonical Monte Carlo. Computer Physics Communications, 1995, 90, 73-80.	7.5	7
22	Cubic and hexagonal symmetries in LiCl nanoclusters. European Physical Journal D, 2007, 44, 109-116.	1.3	7
23	Gibbs ensemble Monte Carlo. American Journal of Physics, 2015, 83, 809-816.	0.7	7
24	Phase behavior of C60 by computer simulation using ab-initio interaction potential. International Journal of Quantum Chemistry, 2001, 84, 375-387.	2.0	5
25	Hypervolume Monte Carlo method at constant pressure. Computer Physics Communications, 1997, 102, 161-165.	7.5	4
26	Prediction of reactive sites for the electropolymerization ofp-benzenesulfonic acid derivatives: Ab initio and experimental study. International Journal of Quantum Chemistry, 2004, 99, 11-27.	2.0	4
27	A time saving algorithm for the Monte Carlo method of Metropolis. Computer Physics Communications, 2006, 175, 116-121.	7.5	4
28	Phase transitions, coexistence and crystal growth dynamics in ionic nanoclusters: Theory and simulation. Computational and Theoretical Chemistry, 2010, 946, 94-106.	1.5	4
29	High dimensional geometry in statistical mechanics. A new microcanonical sampling method. Pure and Applied Chemistry, 1996, 68, 1509-1514.	1.9	3
30	Melting, freezing and nucleation in nanoclusters of potassium chloride. European Physical Journal D, 2008, 47, 373-377.	1.3	3
31	Phase behavior of ionic clusters down to nanoscale. A review of recent work. International Journal of Quantum Chemistry, 2010, 110, 284-292.	2.0	3
32	Improved propagators for the path integral study of quantum systems. Journal of Chemical Physics, 1993, 98, 3300-3305.	3.0	2
33	Phase transitions in ionic clusters. AIP Conference Proceedings, 1995, , .	0.4	1
34	The hypervolume Monte Carlo method at constant pressure applied to liquid methyl chloride. Computational and Theoretical Chemistry, 1999, 463, 157-161.	1.5	1
35	Application of the hypervolume Monte Carlo methods to a molten ionic system. Computational and Theoretical Chemistry, 1999, 463, 191-196.	1.5	1
36	Free energies of ionic nanoclusters. Solid and coexistent solid-liquid states. European Physical Journal D, 2008, 49, 353-359.	1.3	1

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37	Induction of crystal growth in alkali-halide aggregates by means of internal seeding. European Physical Journal D, 2012, 66, 1.	1.3	1
38	Models for the adsorption and selfâ€assembly of ethanol and 1â€decanethiol on Au(111) surfaces. A comparative study by computer simulation. International Journal of Quantum Chemistry, 2010, 110, 293-306.	2.0	0
39	Computer Simulation of Solution/Electrode Interfaces. Portugaliae Electrochimica Acta, 2007, 26, 1-13.	1.1	0
40	Monte Carlo Simulation of the Solvent Contribution to the Potential of Mean Force for the Phenol Adsorption on Au(210) Electrodes. Portugaliae Electrochimica Acta, 2009, 27, 487-503.	1.1	0