Carme Sousa

List of Publications by Year
in descending order

85 papers	2,814 citations	172457 29 h-index	189892 50 g-index
89 all docs	89 docs citations	89 times ranked	2506 citing authors

#	Article	IF	Citations
1	A systematic density functional theory study of the electronic structure of bulk and (001) surface of transition-metals carbides. Journal of Chemical Physics, 2005, 122, 174709.	3.0	180
2	Ultrafast Deactivation Mechanism of the Excited Singlet in the Lightâ€Induced Spin Crossover of [Fe(2,2â€²â€bipyridine)₃]²⁺. Chemistry - A European Journal, 2013, 19, 17541-17551.	3.3	145
3	Multiconfigurational Perturbation Theory:Â An Efficient Tool to Predict Magnetic Coupling Parameters in Biradicals, Molecular Complexes, and Ionic Insulators. Journal of Physical Chemistry A, 2001, 105, 11371-11378.	2.5	129
4	Measures of ionicity of alkaline-earth oxides from the analysis ofab initiocluster wave functions. Physical Review B, 1993, 48, 11573-11582.	3.2	105
5	On modelling the interaction of CO on the MgO(100) surface. Surface Science, 1995, 327, 59-73.	1.9	96
6	Study of the Lightâ€Induced Spin Crossover Process of the [Fe^{II}(bpy)₃]²⁺ Complex. Chemistry - A European Journal, 2010, 16, 4550-4556.	3.3	86
7	Theoretical Approaches to Excited-State-Related Phenomena in Oxide Surfaces. Chemical Reviews, 2013, 113, 4456-4495.	47.7	80
8	Light-Induced Excited-State Spin Trapping in Tetrazole-Based Spin Crossover Systems. Journal of the American Chemical Society, 2008, 130, 13961-13968.	13.7	79
9	Rigorous characterization of oxygen vacancies in ionic oxides. Physical Review B, 2002, 66, .	3.2	75
10	Madelung fields from optimized point charges forab initiocluster model calculations on ionic systems. Journal of Computational Chemistry, 1993, 14, 680-684.	3.3	74
11	Chemisorption of atomic chlorine on metal surfaces and the interpretation of the induced work function changes. Surface Science, 2005, 574, 297-305.	1.9	66
12	Density Functional Study of the Adsorption of Atomic Oxygen on the (001) Surface of Early Transition-Metal Carbides. Journal of Physical Chemistry C, 2007, 111, 1307-1314.	3.1	66
13	Ab initio study of the optical transitions of F centers at low-coordinated sites of the MgO surface. Surface Science, 1999, 429, 217-228.	1.9	64
14	Can corundum be described as an ionic oxide?. Journal of Chemical Physics, 1993, 99, 6818-6823.	3.0	62
15	A Systematic Density Functional Study of Molecular Oxygen Adsorption and Dissociation on the (001) Surface of Group IVâ€“VI Transition Metal Carbides. Journal of Physical Chemistry C, 2007, 111, 16982-16989.	3.1	60
16	Ionic-covalent transition in titanium oxides. Physical Review B, 1994, 50, 13974-13980.	3.2	59
17	Computational approach to the study of thermal spin crossover phenomena. Journal of Chemical Physics, 2014, 140, 184318.	3.0	57
18	Chemical shifts of the core-level binding energies for the alkaline-earth oxides. Chemical Physics Letters, 1992, 196, 641-646.	2.6	53

#	Article	IF	Citations
19	Interaction of oxygen with ZrC(001) and VC(001): Photoemission and first-principles studies. Physical Review B, 2005, 72, .	3.2	50
20	On the prediction of core level binding energies in molecules, surfaces and solids. Physical Chemistry Chemical Physics, 2018, 20, 8403-8410.	2.8	50
21	On the accurate prediction of the optical absorption energy of F-centers in MgO from explicitly correlated ab initio cluster model calculations. Journal of Chemical Physics, 2001, 115, 1435-1439.	3.0	47
22	On the role of the metalâ€toâ€ligand charge transfer states in the lightâ€induced spin crossover in Fe^{II} (bpy)₃. International Journal of Quantum Chemistry, 2011, 111, 3385-3393.	2.0	46
23	Promoter and poisoning effects on NO-catalyzed dissociation on bimetallic RhCu(111) surfaces. Journal of Catalysis, 2006, 239, 431-440.	6.2	45
24	Consequences of electron correlation for XPS binding energies: Representative case for C(1s) and O(1s) XPS of CO. Journal of Chemical Physics, 2016, 145, 144303.	3.0	37
25	Ground- and excited-state properties ofM-center oxygen vacancy aggregates in the bulk and surface of MgO. Physical Review B, 2003, 68, .	3.2	35
26	Optical properties of Cu nanoclusters supported on MgO(100). Journal of Chemical Physics, 2004, 121, 7457-7466.	3.0	35
27	Assessing the zero-field splitting in magnetic molecules by wave function-based methods. International Journal of Quantum Chemistry, 2006, 106, 2470-2478.	2.0	35
28	Correcting Flaws in the Assignment of Nitrogen Chemical Environments in N-Doped Graphene. Journal of Physical Chemistry C, 2019, 123, 11319-11327.	3.1	33
29	The effect of local environment on photoluminescence: A time-dependent density functional theory study of silanone groups on the surface of silica nanostructures. Journal of Chemical Physics, 2009, 131, 034705.	3.0	32
30	Optical properties of peroxy radicals in silica: Multiconfigurational perturbation theory calculations. Journal of Chemical Physics, 2001, 114, 6259-6264.	3.0	31
31	Ionization and excitation energies in CuCl and NiO within different embedding schemes. Computational and Theoretical Chemistry, 1998, 458, 53-60.	1.5	30
32	Theoretical Study of the Interaction of Molecular Hydrogen with PdCu(111) Bimetallic Surfaces. Journal of Physical Chemistry B, 2001, 105, 1817-1822.	2.6	29
33	First-principles study of the optical transitions ofFcenters in the bulk and on the (0001) surface ofÎ±â^'Al2O3. Physical Review B, 2005, 72, .	3.2	29
34	Optical absorption and luminescence energies of F centers in CaO fromab initioembedded cluster calculations. Journal of Chemical Physics, 2006, 125, 074710.	3.0	29
35	Theoretical evidence for the direct ³MLCT-HS deactivation in the light-induced spin crossover of Fe(<scp>ii</scp>)â€"polypyridyl complexes. Physical Chemistry Chemical Physics, 2018, 20, 2351-2355.	2.8	29
36	Coherent tunneling inCu2+- andAg2+-doped MgO andCaO:Cu2+explored throughab initiocalculations. Physical Review B, 2005, 72, .	3.2	27

#	Article	IF	Citations
37	Theoretical Study of the Catalytic Activity of Bimetallic RhCu Surfaces and Nanoparticles toward H2 Dissociation. Journal of Physical Chemistry B, 2002, 106, 7839-7845.	2.6	26
38	Effect of the surface model on the theoretical description of the chemisorption of atomic hydrogen on Cu(). Surface Science, 2003, 522, 185-197.	1.9	26
39	Excited states of MgO: A cluster model study. Journal of Chemical Physics, 1994, 100, 2943-2946.	3.0	25
40	Theoretical study of the chemisorption of CO on bimetallic RhCu surfaces and nanoparticles. Surface Science, 2003, 531, 39-52.	1.9	25
41	Combining molecular dynamics and ab initio quantum-chemistry to describe electron transfer reactions in electrochemical environments. Journal of Chemical Physics, 2004, 121, 1066-1073.	3.0	25
42	Topological analysis of charge density in ionic solids. Chemical Physics Letters, 1993, 215, 97-102.	2.6	23
43	Electrostatic and chemical bonding contributions to the cation core level binding energy shifts in MgO, CaO, SrO, BaO. A cluster model study. Journal of Electron Spectroscopy and Related Phenomena, 1993, 63, 189-205.	1.7	23
44	Theoretical Study of the Light-Induced Spin Crossover Mechanism in [Fe(mtz)₆]²⁺ and [Fe(phen)₃]²⁺. Journal of Physical Chemistry A, 2017, 121, 9720-9727.	2.5	23
45	Theoretical Study of CO and NO Chemisorption on RhCu(111) Surfaces. Journal of Physical Chemistry B, 2005, 109, 4654-4661.	2.6	21
46	Electric field effects on the ionic-neutral curve crossing of alkali halide molecules. Journal of Chemical Physics, 2000, 113, 9940-9947.	3.0	20
47	Theoretical characterization of the low-lying excited states of the CuCl molecule. Journal of Chemical Physics, 1997, 106, 7162-7169.	3.0	19
48	Effect of Secondâ€Order Spinâ€“Orbit Coupling on the Interaction between Spin States in Spinâ€Crossover Systems. Chemistry - A European Journal, 2018, 24, 5146-5152.	3.3	19
49	Deactivation of Excited States in Transitionâ€Metal Complexes: Insight from Computational Chemistry. Chemistry - A European Journal, 2019, 25, 1152-1164.	3.3	19
50	Neutral atoms in ionic lattices:â€ƒExcited states ofKCl:Ag0. Physical Review B, 2000, 62, 13366-13375.	3.2	18
51	The fate of optical excitations in small polyhedral ZnS clusters: A theoretical study of the excitation and localization of electrons in Zn4S4and Zn6S6. Journal of Chemical Physics, 2011, 134, 064511.	3.0	18
52	Core exciton energies of bulk MgO,Al2O3,andSiO2from explicitly correlatedab initiocluster model calculations. Physical Review B, 2000, 62, 10013-10021.	3.2	17
53	Ab initiostudy of the charge order and Zener polaron formation in half-doped manganites. Physical Review B, 2004, 70, .	3.2	17
54	Hopping matrix elements from first-principles studies of overlapping fragments: Double exchange parameters in manganites. International Journal of Quantum Chemistry, 2006, 106, 2444-2457.	2.0	16

#	Article	IF	Citations
55	The effect of thermal motion on the electron localization in metal-to-ligand charge transfer excitations in [Fe(bpy)₃]²⁺. Dalton Transactions, 2014, 43, 17838-17846.	3.3	16
56	Role of surface heterogeneity in the chemical bond of MgO: ionic character of regular and defect surface sites. Chemical Physics Letters, 1996, 249, 123-129.	2.6	15
57	Explanation of the site-specific spin crossover in Fe(mtz)6(BF4)2. Dalton Transactions, 2013, 42, 14702.	3.3	15
58	Theoretical evidence for the existence of excitons in MgO. Chemical Physics Letters, 1995, 239, 263-266.	2.6	13
59	Is it possible to use Charge Transfer Bands to Measure Impurity-Ligand Distances? Experimental and Theoretical Results on Cu 2+ Doped (C 2 H 5 NH 3) 2 CdCl 4. High Pressure Research, 2002, 22, 475-478.	1.2	13
60	Neutral atoms in ionic lattices:â€ƒStability and ground-state properties ofKCl:Ag0. Physical Review B, 2000, 62, 13356-13365.	3.2	12
61	Valence bond reading of ab initio molecular orbital cluster model wavefunctions: the nature of chemical bond in corundum. Journal of Electron Spectroscopy and Related Phenomena, 1994, 69, 65-71.	1.7	11
62	Ab initiotheory of magnetic interactions at surfaces. Journal of Physics Condensed Matter, 2004, 16, S2557-S2574.	1.8	11
63	Similarities and differences on the molecular mechanism of CO oxidation on Rh(111) and bimetallic RhCu(111) surfaces. Physical Chemistry Chemical Physics, 2007, 9, 2877-2885.	2.8	11
64	Optical excitations of defects in realistic nanoscale silica clusters: Comparing the performance of density functional theory using hybrid functionals with correlated wavefunction methods. Journal of Chemical Physics, 2008, 129, 014706.	3.0	11
65	Optical spectroscopy of (C2H5NH3)2CdCl4:Cu2+under pressure: Study of Cu2+local structure from theoretical calculations. International Journal of Quantum Chemistry, 2002, 86, 239-244.	2.0	9
66	Assessing the ability of DFT methods to describe static electron correlation effects: CO core level binding energies as a representative case. Journal of Chemical Physics, 2017, 147, 024106.	3.0	9
67	On the role of dynamic electron correlation in non-orthogonal configuration interaction with fragments. Physical Chemistry Chemical Physics, 2022, 24, 11931-11944.	2.8	9
68	Electric field effects in the chemisorption of CO on bimetallic RhCu surface models. Surface Science, 2004, 548, 209-219.	1.9	8
69	The Role of Vibrational Anharmonicity in the Computational Study of Thermal Spin Crossover. Magnetochemistry, 2019, 5, 49.	2.4	8
70	GronOR: Scalable and Accelerated Nonorthogonal Configuration Interaction for Molecular Fragment Wave Functions. Journal of Chemical Theory and Computation, 2022, 18, 3549-3565.	5.3	8
71	Ab initio study of the optical transitions on low-coordinated sites of an intermediate F center: The Fs+(OH)â^' center on MgO(100) surface. Solid State Ionics, 2007, 178, 173-178.	2.7	7
72	FEATURES AND CATALYTIC PROPERTIES OF RhCu: A REVIEW. International Journal of Modern Physics B, 2010, 24, 5128-5138.	2.0	7

#	Article	IF	Citations
73	Differential many-body effects for initial and core ionic states: impact on XPS spectra. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	7
74	Character of the electronic ground state and of charge-transfer excited states in ionic solids: An ab initio cluster model approach. International Journal of Quantum Chemistry, 1994, 52, 281-293.	2.0	6
75	Electric field induced electron transfer at the adsorbateâ€“surface interface. Effect of the type of metal surface. Physical Chemistry Chemical Physics, 2005, 7, 3353.	2.8	6
76	A Quantum Chemical Model for Electric Field Induced Electron Transfer at Metal Electrodes. Application to Halide Oxidation on Cu(100). Journal of Physical Chemistry B, 2002, 106, 12483-12490.	2.6	5
77	Limitations of the equivalent core model for understanding core-level spectroscopies. Physical Chemistry Chemical Physics, 2020, 22, 22617-22626.	2.8	5
78	Elementary Steps of Catalytic Processes on Metallic and Bimetallic Surfaces. Progress in Theoretical Chemistry and Physics, 2001, , 149-181.	0.2	5
79	Consequences of chemical bonding on the adiabaticity of gas-surface reactions. Computational and Theoretical Chemistry, 1996, 371, 257-267.	1.5	4
80	Effect of electron correlation in the decomposition of core level binding energy shifts into initial and final state contributions. Physical Chemistry Chemical Physics, 2019, 21, 9399-9406.	2.8	4
81	Approaching multiplet splitting in X-ray photoelectron spectra by density functional theory methods: NO and O2 molecules as examples. Chemical Physics Letters, 2019, 731, 136617.	2.6	3
82	Excited States in Metal Oxides by Configuration Interaction and Multireference Perturbation Theory. Progress in Theoretical Chemistry and Physics, 2000, , 227-245.	0.2	3
83	Reliability of atomic natural orbital basis sets in calculations involving pseudopotentials. Journal of Computational Chemistry, 1992, 13, 148-154.	3.3	0
84	Stability and optical properties of silver atoms in KCl. Radiation Effects and Defects in Solids, 2001, 154, 249-253.	1.2	0
85	The Ground and Excited States of Oxides. , 2002, , 93-109.		0