Pietro Cortona

List of Publications by Year
in descending order

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50	1,839	394390	254170
papers	citations	19	43
		h-index	g-index

51	51	51	1888
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Self-consistently determined properties of solids without band-structure calculations. Physical Review B, 1991, 44, 8454-8458.	3.2	381
2	On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. Journal of Chemical Theory and Computation, 2013, 9, 3118-3126.	5.3	335
3	Direct determination of self-consistent total energies and charge densities of solids: A study of the cohesive properties of the alkali halides. Physical Review B, 1992, 46, 2008-2014.	3.2	138
4	Communication: One third: A new recipe for the PBE0 paradigm. Journal of Chemical Physics, 2013, 138, 021104.	3.0	115
5	Effective electron displacements: A tool for time-dependent density functional theory computational spectroscopy. Journal of Chemical Physics, 2014, 140, 104101.	3.0	63
6	An ab-initio study of the rÃ1e of lone pairs in the structure and insulatorâ€“metal transition in SnO and PbO. Solid State Sciences, 2002, 4, 467-474.	3.2	61
7	A new parameter-free correlation functional based on an average atomic reduced density gradient analysis. Journal of Chemical Physics, 2008, 128, 034101.	3.0	56
8	Large thermal conductivity decrease in point defective Bi2Te3 bulk materials and superlattices. Journal of Applied Physics, 2013, 113, .	2.5	54
9	Cohesive properties and behaviour under pressure of CaS, CaSe, and CaTe: results ofab initiocalculations. Journal of Physics Condensed Matter, 1998, 10, 8947-8955.	1.8	52
10	Semiclassical atom theory applied to solid-state physics. Physical Review B, 2016, 93, .	3.2	51
11	Classical to Quantum Transition of Heat Transfer between Two Silica Clusters. Physical Review Letters, 2014, 112, 114301.	7.8	44
12	Ab initiocalculations of cohesive and structural properties of the alkali-earth oxides. Journal of Physics Condensed Matter, 1996, 8, 8983-8994.	1.8	36
13	Note: Theoretical mixing coefficients for hybrid functionals. Journal of Chemical Physics, 2012, 136, 086101.	3.0	36
14	Correlation energy of many-electron systems: A modified Colleâ€“Salvetti approach. Journal of Chemical Physics, 2004, 121, 7671.	3.0	33
15	Increasing physical constraints and improving performances in a parameter-free GGA functional. Chemical Physics Letters, 2008, 460, 536-539.	2.6	33
16	New self-interaction-corrected local-density approximation to the density-functional theory. Physical Review A, 1986, 34, 769-776.	2.5	31
17	Toward a Combined DFT/QTAIM Description of Agostic Bonds: The Critical Case of a Nb(III) Complex. Journal of Physical Chemistry A, 2009, 113, 12322-12327.	2.5	31
18	Ab-initio study of the structural phase transition of SrSe and SrTe under pressure. International Journal of Quantum Chemistry, 2004, 99, 828-832.	2.0	22

#	Article	IF	Citations
19	Global Hybrids from the Semiclassical Atom Theory Satisfying the Local Density Linear Response. Journal of Chemical Theory and Computation, 2015, 11, 122-131.	5.3	22
20	The performances of a parameter-free local correlation functional: The Ragotâ€“Cortona model. Chemical Physics Letters, 2007, 439, 381-385.	2.6	19
21	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. Computation, 2018, 6, 7.	2.0	17
22	Interconfigurational energies and ionization potentials: Test of a correlation energy functional. Chemical Physics, 2007, 337, 161-167.	1.9	16
23	Activation enthalpies of pericyclic reactions: the performances of some recently proposed functionals. Theoretical Chemistry Accounts, 2009, 122, 257-264.	1.4	16
24	Self-consistent calculations of total energies and charge densities of solids without solving the band-structure problem. International Journal of Quantum Chemistry, 1994, 52, 987-992.	2.0	14
25	Generalized gradient exchange functionals based on the gradient-regulated connection: a new member of the TCA family. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	14
26	Assessing modern GGA functionals for solids. Journal of Molecular Modeling, 2013, 19, 2791-2796.	1.8	14
27	Analysis of the MgO structure factors. Physical Review B, 1999, 60, 8569-8574.	3.2	13
28	Assessing the performances of some recently proposed density functionals for the description of bond dissociations involving organic radicals. International Journal of Quantum Chemistry, 2010, 110, 2320-2329.	2.0	12
29	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	12
30	Complementary aspects of charge and momentum density for the study of the chemical bond. Theoretical Chemistry Accounts, 2001, 105, 284-291.	1.4	10
31	Density-functional calculations for large systems: Can GGA functionals Be competitive with hybrid functionals?. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 163-168.	3.6	10
32	Stability of the different AlOOH phases under pressure. Journal of Physics Condensed Matter, 2016, 28, 185401.	1.8	10
33	Hydrogen bond symmetrization and elastic constants under pressure ofÎ´-AlOOH. Journal of Physics Condensed Matter, 2017, 29, 325505.	1.8	10
34	Self-interaction correction: The transition-metal atoms. Physical Review A, 1988, 38, 3850-3856.	2.5	7
35	The (100), (110), and (111) Cu surfaces revisited by the semiempirical LCAO method. International Journal of Quantum Chemistry, 2004, 99, 713-723.	2.0	7
36	Exchange energy in density-functional theory:â€ƒA nonlocal approximation based on a self-consistent determination of the Î± parameter of the SlaterXÎ±theory. Physical Review A, 1998, 57, 4306-4310.	2.5	6

#	Article	IF	Citations
37	Simplified method for fully relativistic spin-polarized density-functional calculations. Physical Review B, 1989, 40, 12105-12110.	3.2	5
38	LCAO study of the Cu(110)-p(2Ã—1)O surface. Surface Science, 2005, 585, 155-162.	1.9	5
39	New Correlation Functionals In DFT: Theory And Tests. , 2009, , .		5
40	New range-separated hybrids based on the TCA density functional. Chemical Physics Letters, 2012, 519-520, 145-149.	2.6	5
41	Dispersion corrections applied to the TCA family of exchange-correlation functionals. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	4
42	Transverse exchange energy in relativistic density-functional calculations: An alternative approximation. Physical Review A, 1994, 49, 825-828.	2.5	3
43	Semi-empirical LCAO analysis of the surface states of Cu: the () surface. Surface Science, 2003, 532-535, 19-24.	1.9	3
44	Electronic structure of the Cu-p(2Ã—1)O surface by the semi-empirical LCAO method. Surface Science, 2004, 566-568, 1102-1106.	1.9	3
45	Investigation of the surface bands along theXÂ¯â^'MÂ¯line of the Cu(100) surface. Physical Review B, 2007, 75, .	3.2	3
46	Towards a Greater Accuracy in DFT Calculations: From GGA to Hybrid Functionals. , 2012, , 3-15.		1
47	Ab initio calculations of ideal and defective bismuth telluride nanotubes. Physica Status Solidi (B): Basic Research, 2015, 252, 517-520.	1.5	1
48	Generalized gradient exchange functionals based on the gradient-regulated connection: a new member of the TCA family. Highlights in Theoretical Chemistry, 2013, , 237-243.	0.0	0
49	Overview of the Degeneracy-Dependent Self-Interaction Correction (D-SIC). , 1991, , 307-321.		0
50	Relativistic Spin-Polarized Density-Functional Theory: Simplified Method for Fully Relativistic Calculations. , 1991, , 285-293.		0