Pietro Cortona

List of Publications by Citations

50 papers	1,574 citations	19 h-index	39 g-index
51 ext. papers	1,711 ext. citations	2.8 avg, IF	4.85 L-index

#	Paper	IF	Citations
50	Self-consistently determined properties of solids without band-structure calculations. *Physical Review B*, **1991**, 44, 8454-8458	3.3	344
49	On the Metric of Charge Transfer Molecular Excitations: A Simple Chemical Descriptor. *Journal of Chemical Theory and Computation*, **2013**, 9, 3118-26	6.4	247
48	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	3.3	126
47	Communication: one third: a new recipe for the PBE0 paradigm. *Journal of Chemical Physics*, **2013**, 138, 021104	3.9	84
46	An ab-initio study of the rle of lone pairs in the structure and insulatormetal transition in SnO and PbO. *Solid State Sciences*, **2002**, 4, 467-474	3.4	53
45	Effective electron displacements: a tool for time-dependent density functional theory computational spectroscopy. *Journal of Chemical Physics*, **2014**, 140, 104101	3.9	50
44	Semiclassical atom theory applied to solid-state physics. *Physical Review B*, **2016**, 93,	3.3	49
43	A new parameter-free correlation functional based on an average atomic reduced density gradient analysis. *Journal of Chemical Physics*, **2008**, 128, 034101	3.9	49
42	Large thermal conductivity decrease in point defective Bi2Te3 bulk materials and superlattices. *Journal of Applied Physics*, **2013**, 113, 013506	2.5	48
41	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	45
40	Classical to quantum transition of heat transfer between two silica clusters. *Physical Review Letters*, **2014**, 112, 114301	7.4	33
39	Note: Theoretical mixing coefficients for hybrid functionals. *Journal of Chemical Physics*, **2012**, 136, 086101	3.9	33
38	Ab initiocalculations of cohesive and structural properties of the alkali-earth oxides. *Journal of Physics Condensed Matter*, **1996**, 8, 8983-8994	1.8	33
37	Increasing physical constraints and improving performances in a parameter-free GGA functional. *Chemical Physics Letters*, **2008**, 460, 536-539	2.5	31
36	Correlation energy of many-electron systems: a modified Colle-Salvetti approach. *Journal of Chemical Physics*, **2004**, 121, 7671-80	3.9	31
35	Toward a combined DFT/QTAIM description of agostic bonds: the critical case of a Nb(III) complex. *Journal of Physical Chemistry A*, **2009**, 113, 12322-7	2.8	30
34	New self-interaction-corrected local-density approximation to the density-functional theory. *Physical Review A*, **1986**, 34, 769-776	2.6	30

33	Ab-initio study of the structural phase transition of SrSe and SrTe under pressure. *International Journal of Quantum Chemistry*, **2004**, 99, 828-832	2.1	21
32	Global hybrids from the semiclassical atom theory satisfying the local density linear response. *Journal of Chemical Theory and Computation*, **2015**, 11, 122-31	6.4	20
31	The performances of a parameter-free local correlation functional: The Ragot□ortona model. *Chemical Physics Letters*, **2007**, 439, 381-385	2.5	19
30	Activation enthalpies of pericyclic reactions: the performances of some recently proposed functionals. *Theoretical Chemistry Accounts*, **2009**, 122, 257-264	1.9	15
29	Interconfigurational energies and ionization potentials: Test of a correlation energy functional. *Chemical Physics*, **2007**, 337, 161-167	2.3	15
28	Solid-State Testing of a Van-Der-Waals-Corrected Exchange-Correlation Functional Based on the Semiclassical Atom Theory. *Computation*, **2018**, 6, 7	2.2	14
27	Assessing modern GGA functionals for solids. *Journal of Molecular Modeling*, **2013**, 19, 2791-6	2	13
26	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	2.1	13
25	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	12
24	Generalized gradient exchange functionals based on the gradient-regulated connection: a new member of the TCA family. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	12
23	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	2.1	11
22	Complementary aspects of charge and momentum density for the study of the chemical bond. *Theoretical Chemistry Accounts*, **2001**, 105, 284-291	1.9	10
21	Analysis of the MgO structure factors. *Physical Review B*, **1999**, 60, 8569-8574	3.3	10
20	Density-functional calculations for large systems: can GGA functionals be competitive with hybrid functionals?. *Interdisciplinary Sciences, Computational Life Sciences*, **2010**, 2, 163-8	3.5	9
19	The (100), (110), and (111) Cu surfaces revisited by the semiempirical LCAO method. *International Journal of Quantum Chemistry*, **2004**, 99, 713-723	2.1	7
18	Self-interaction correction: The transition-metal atoms. *Physical Review A*, **1988**, 38, 3850-3856	2.6	7
17	Exchange energy in density-functional theory: A nonlocal approximation based on a self-consistent determination of the □parameter of the Slater X□theory. *Physical Review A*, **1998**, 57, 4306-4310	2.6	6
16	Hydrogen bond symmetrization and elastic constants under pressure of □AlOOH. *Journal of Physics Condensed Matter*, **2017**, 29, 325505	1.8	5

15	New range-separated hybrids based on the TCA density functional. *Chemical Physics Letters*, **2012**, 519-520, 145-149	2.5	5
14	New Correlation Functionals In DFT: Theory And Tests **2009**,		5
13	LCAO study of the Cu(110)-p(2×1)O surface. *Surface Science*, **2005**, 585, 155-162	1.8	5
12	Simplified method for fully relativistic spin-polarized density-functional calculations. *Physical Review B*, **1989**, 40, 12105-12110	3.3	5
11	Stability of the different AlOOH phases under pressure. *Journal of Physics Condensed Matter*, **2016**, 28, 185401	1.8	4
10	Investigation of the surface bands along the X□M□ line of the Cu(100) surface. *Physical Review B*, **2007**, 75,	3.3	3
9	Electronic structure of the Cu-p(2×1)O surface by the semi-empirical LCAO method. *Surface Science*, **2004**, 566-568, 1102-1106	1.8	3
8	Semi-empirical LCAO analysis of the surface states of Cu: the () surface. *Surface Science*, **2003**, 532-535, 19-24	1.8	3
7	Transverse exchange energy in relativistic density-functional calculations: An alternative approximation. *Physical Review A*, **1994**, 49, 825-828	2.6	3
6	Dispersion corrections applied to the TCA family of exchange-correlation functionals. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	2
5	Ab initio calculations of ideal and defective bismuth telluride nanotubes. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 517-520	1.3	1
4	Towards a Greater Accuracy in DFT Calculations: From GGA to Hybrid Functionals **2012**, 3-15		
3	Overview of the Degeneracy-Dependent Self-Interaction Correction (D-SIC) **1991**, 307-321		
2	Relativistic Spin-Polarized Density-Functional Theory: Simplified Method for Fully Relativistic Calculations **1991**, 285-293		
1	Generalized gradient exchange functionals based on the gradient-regulated connection: a new member of the TCA family. *Highlights in Theoretical Chemistry*, **2013**, 237-243		