Marie-Bernadette Lepetit

List of Publications by Year
in descending order

50	1,046	394286	414303
papers	citations	19 h-index	32 g-index

50	50	50	1401
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Large Increase of the Curie Temperature by Orbital Ordering Control. Physical Review Letters, 2010, 104, 046804.	2.9	89
2	Fast calculation of the electrostatic potential in ionic crystals by direct summation method. Journal of Chemical Physics, 2008, 128, 244716.	1.2	72
3	Evidence for Room Temperature Electric Polarization in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>R</mml:mi><mml:mi mathvariant="normal">M</mml:mi><mml:mi mathvariant="normal">n</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:msub><mml:m mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>5</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:	2.9	60
4	Ab initioevaluation of local effective interactions inÎ±â€²â^'NaV2O5. Physical Review B, 2000, 62, 402-409.	1.1	59
5	Importance of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>t</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mi>g</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> in transition metal oxides. Physical Review B, 2008, 77, .	1.1	56
6	Interface Effects in Perovskite Thin Films. Physical Review Letters, 2012, 108, 087202.	2.9	52
7	Ab InitioEvaluation of the Charge Ordering inÎ±â€²NaV2O5. Physical Review Letters, 2002, 88, 056405.	2.9	51
8	Orbital-Ordering-Driven Multiferroicity and Magnetoelectric Coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>GeV</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub><mml:msub><mml:m mathvariant="normal">S</mml:mi></mml:mrow><mml:mrow><mml:mn>8</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:m Physical Review Letters, 2014, 113, 137602.	2.9	51
9	Origins of the poor convergence of manyâ€body perturbation theory expansions from unrestricted Hartreeâ€“Fock zerothâ€order descriptions. Journal of Chemical Physics, 1988, 89, 998-1008.	1.2	38
10	Abinitioevaluation of the local effective interactions in the superconducting compoundNa0.35CoO2â^™1.3H2O. Physical Review B, 2006, 74, .	1.1	37
11	Leading interactions in theÎ²â^'SrV6O15compound. Physical Review B, 2005, 71, .	1.1	34
12	Role of dynamical polarization of the ligand-to-metal charge transfer excitations inab initiodetermination of effective exchange parameters. Physical Review B, 2003, 68, .	1.1	31
13	Influence of the Incommensurability inSr14â^'xCaxCu24O41Family Compounds. Physical Review Letters, 2004, 92, 236402.	2.9	29
14	Elastic and magnetic effects on the infrared phonon spectra of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MnF</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2010, 82, .	1.1	28
15	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>Co<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	1.1	28
16	Environment effects on effective magnetic exchange integrals and local spectroscopy of extended strongly correlated systems. Journal of Chemical Physics, 2003, 118, 3966-3973.	1.2	24
17	Multiferroicity and magnetoelastic coupling in Î±â^'Mn2O3 : A binary perovskite. Physical Review B, 2018, 98, .	1.1	23
18	Magnetic coupling and long-range order in the spinâ€“chain sulfide Ba2CoS3. Journal of Materials Chemistry, 2006, 16, 3489-3502.	6.7	22

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19	Spin-orbital nature of the high-field magnetic state in theSr4Ru3O10. Physical Review B, 2016, 93, .	1.1	21
20	Multiplicity of symmetry-broken Hartree-Fock solutions in multiple bonds and atomic clusters: An asymptotic view. Physical Review A, 1989, 39, 981-991.	1.0	19
21	From one-electron to correlated wave functions in extended systems: A valence-bond investigation. Physical Review A, 1989, 39, 3274-3288.	1.0	18
22	Dimerization of polyacetylene using a distance-dependent Hubbard model and the density-matrix renormalization-group method. Physical Review B, 1997, 56, 4447-4454.	1.1	18
23	Anab initiostudy of magneto-electric coupling of YMnO₃. Journal of Physics Condensed Matter, 2013, 25, 496004.	0.7	18
24	Investigation of the electromagnon excitations in the multiferroic TbMn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, .	1.1	17
25	Real-space renormalization-group studies of low-dimensional quantum antiferromagnets. Physical Review B, 1993, 48, 1028-1035.	1.1	16
26	Toward a magnetic description of metals in terms of interstitial molecular orbitals: Exploiting the multiplicity of symmetry-broken Hartree-Fock solutions on small alkali-metal clusters. Physical Review B, 1990, 41, 8093-8106.	1.1	15
27	Toward a magnetic description of metals in terms of interstitial molecular orbitals. II. One-dimensional infinite system: The lithium chain. Physical Review B, 1992, 46, 12974-12980.	1.1	13
28	Simple generation of an approximate internally correlated wave function from the Hartree-Fock approximation and its valence-bond decomposition. Physical Review A, 1989, 39, 3289-3297.	1.0	11
29	Analysis of the multiferroicity in the hexagonal manganite YMnO3. Journal of Physics Condensed Matter, 2013, 25, 416002.	0.7	10
30	Combined First-Principles Calculations and Experimental Study of the Phonon Modes in the Multiferroic Compound GeV₄S₈. Journal of Physical Chemistry C, 2017, 121, 3522-3529.	1.5	10
31	Room temperature polar structure and multiferroicity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>BaFe</mml:mi><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub><mml:mi>Se</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2020, 101, .	1.1	9
32	Current-current correlations in aCuO3model system. Physical Review B, 2002, 66, .	1.1	8
33	Correlation and dimerization effects on the physical behavior of the NR4[Ni(dmit)2]2 charge transfer salts: A density matrix renormalization group study of the quarter-filling tâ€“J model. Journal of Chemical Physics, 1999, 110, 1767-1773.	1.2	6
34	Optical phonons in a quarter-filled one-dimensional Hubbard model. Physical Review B, 2000, 62, 10744-10751.	1.1	6
35	Phonons in the multiferroic langasiteBa3NbFe3Si2O14: Evidence for symmetry breaking. Physical Review B, 2015, 92, .	1.1	6
36	Parity law of the singlet-triplet gap in graphitic ribbons. European Physical Journal B, 2006, 51, 517-522.	0.6	5

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37	Influence of structural modulations and the chain-ladder interaction in theSr14âˆ'xCaxCu24O41compounds. Physical Review B, 2006, 74, .	1.1	5
38	Evidence for an electromagnon in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>GdMn</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mathvariant="normal">O</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math> : A multiferroic with a large electric polarization. Physical Review B, 2021, 103, .	1.1	5
39	How to compute the magneto-electric tensor from ab-initio calculations?. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	4
40	Anab initioevaluation of the local effective interactions in the NaxCoO2family. Journal of Physics Condensed Matter, 2010, 22, 345603.	0.7	3
41	Control of the orbital ordering in manganite superlattices and impact on properties. Physical Review B, 2017, 96, .	1.1	3
42	For an ab initio calculation of the magnetic excitations: RelaxSE!. Journal of Chemical Physics, 2021, 154, 164116.	1.2	3
43	Interstitial Orbitals for Simple Metals:Â 2D Systems. The Journal of Physical Chemistry, 1996, 100, 4224-4228.	2.9	2
44	Density-matrix renormalization using three classes of block states. Physical Review B, 1998, 58, 12691-12698.	1.1	2
45	Effective valence-bond theory for strongly correlated systems. Computational and Theoretical Chemistry, 2017, 1116, 59-63.	1.1	2
46	Pressure-dependent X-ray diffraction of the multiferroics RMn₂O₅. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 687-696.	0.5	2
47	Theoretical study of the magnetic properties of BaNiF$$_4$$. European Physical Journal B, 2021, 94, 1.	0.6	2
48	Lattice dynamics of BaFe₂Se₃. Journal of Physics Condensed Matter, 2022, 34, 255402.	0.7	2
49	Effect of nearest neighbor repulsion on the low-frequency phase diagram of a quarter-filled Hubbard-Holstein chain. Physical Review B, 2002, 66, .	1.1	1
50	Bond-Order-Wave versus Spin-Density-Wave Dimerization in Polyacetylene. , 1998, , 45-52.		0