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	Lattice dynamics of BaFe₂Se₃. Journal of Physics Condensed Matter, 2022, 34, 255402.	0.7	2
2	For an ab initio calculation of the magnetic excitations: RelaxSE!. Journal of Chemical Physics, 2021, 154, 164116.	1.2	3
3	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
4	Theoretical study of the magnetic properties of BaNiF$$_4$$. European Physical Journal B, 2021, 94, 1.	0.6	2
5	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
6	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
7	Multiferroicity and magnetoelastic coupling in Î±âˆ'Mn2O3 : A binary perovskite. Physical Review B, 2018, 98, .	1.1	23
8	Effective valence-bond theory for strongly correlated systems. Computational and Theoretical Chemistry, 2017, 1116, 59-63.	1.1	2
9	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
10	Control of the orbital ordering in manganite superlattices and impact on properties. Physical Review B, 2017, 96, .	1.1	3
11	How to compute the magneto-electric tensor from ab-initio calculations?. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	4
12	Spin-orbital nature of the high-field magnetic state in theSr4Ru3O10. Physical Review B, 2016, 93, .	1.1	21
13	Phonons in the multiferroic langasiteBa3NbFe3Si2O14: Evidence for symmetry breaking. Physical Review B, 2015, 92, .	1.1	6
14	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:mi>O</mml:mi><mml:mrow><mml:mn>5</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Multiferroics. Physical Review Letters, 2014, 113, 137602.	2.9	60
15	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:mathvariant="normal">S</mml:mi></mml:mrow><mml:mrow><mml:mn>8</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review Letters, 2014, 113, 137602.	7.9	51
16	Anab initiostudy of magneto-electric coupling of YMnO₃. Journal of Physics Condensed Matter, 2013, 25, 496004.	0.7	18
17	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
18	Analysis of the multiferroicity in the hexagonal manganite YMnO3. Journal of Physics Condensed Matter, 2013, 25, 416002.	0.7	10

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19	Interface Effects in Perovskite Thin Films. Physical Review Letters, 2012, 108, 087202.	2.9	52
20	Electronic structure of the Ca<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 /><mml:	1.1	28
21	Large Increase of the Curie Temperature by Orbital Ordering Control. Physical Review Letters, 2010, 104, 046804.	2.9	89
22	Anab initioevaluation of the local effective interactions in the NaxCoO2family. Journal of Physics Condensed Matter, 2010, 22, 345603.	0.7	3
23	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:msub></mml:mrow></mml:math>. Physical Review B, 2010, 82, .	1.1	28
24	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	76
25	Fast calculation of the electrostatic potential in ionic crystals by direct summation method. Journal of Chemical Physics, 2008, 128, 244716.	1.2	72
26	Magnetic coupling and long-range order in the spinâ€“chain sulfide Ba2CoS3. Journal of Materials Chemistry, 2006, 16, 3489-3502.	6.7	22
27	Parity law of the singlet-triplet gap in graphitic ribbons. European Physical Journal B, 2006, 51, 517-522.	0.6	5
28	Influence of structural modulations and the chain-ladder interaction in theSr14âˆ’xCaxCu24O41compounds. Physical Review B, 2006, 74, .	1.1	5
29	Abinitioevaluation of the local effective interactions in the superconducting compoundNa0.35CoO2âˆ™1.3H2O. Physical Review B, 2006, 74, .	1.1	37
30	Leading interactions in theÎ²âˆ’SrV6O15compound. Physical Review B, 2005, 71, .	1.1	34
31	Influence of the Incommensurability inSr14âˆ’xCaxCu24O41Family Compounds. Physical Review Letters, 2004, 92, 236402.	2.9	29
32	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
33	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
34	Ab InitioEvaluation of the Charge Ordering inÎ±â€²NaV2O5. Physical Review Letters, 2002, 88, 056405.	2.9	51
35	Current-current correlations in aCuO3model system. Physical Review B, 2002, 66, .	1.1	8
36	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

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37	Optical phonons in a quarter-filled one-dimensional Hubbard model. Physical Review B, 2000, 62, 10744-10751.	1.1	6
38	Ab initioevaluation of local effective interactions inÎ±â€²â€”NaV2O5. Physical Review B, 2000, 62, 402-409.	1.1	59
39	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
40	Density-matrix renormalization using three classes of block states. Physical Review B, 1998, 58, 12691-12698.	1.1	2
41	Bond-Order-Wave versus Spin-Density-Wave Dimerization in Polyacetylene. , 1998, , 45-52.		0
42	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
43	Interstitial Orbitals for Simple Metals:Â 2D Systems. The Journal of Physical Chemistry, 1996, 100, 4224-4228.	2.9	2
44	Real-space renormalization-group studies of low-dimensional quantum antiferromagnets. Physical Review B, 1993, 48, 1028-1035.	1.1	16
45	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
46	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
47	From one-electron to correlated wave functions in extended systems: A valence-bond investigation. Physical Review A, 1989, 39, 3274-3288.	1.0	18
48	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
49	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
50	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