Myrta GrÃ¼ning

List of Publications by Year
in descending order

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48 papers	3,392 citations	257450 24 h-index	223800 46 g-index
50 all docs	50 docs citations	50 times ranked	3620 citing authors

#	Article	IF	Citations
1	Optical response and band structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LiCoO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> including electron-hole interaction effects. Physical Review B, 2021, 104, .	3.2	18
2	Thermal conductivity of porous polycrystalline PbTe. Physical Review Materials, 2021, 5, .	2.4	0
3	Electronic structure of chromium trihalides beyond density functional theory. Physical Review B, 2021, 104, .	3.2	18
4	Double k-Grid Method for Solving the Bethe-Salpeter Equation via Lanczos Approaches. Frontiers in Chemistry, 2021, 9, 763946.	3.6	2
5	Towards temperature-induced topological phase transition in SnTe: A first-principles study. Physical Review B, 2020, 101, .	3.2	9
6	Role of the lattice in the light-induced insulator-to-metal transition in vanadium dioxide. Physical Review Research, 2020, 2, .	3.6	9
7	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> study of pressure-induced topological insulator transition in group-IV tellurides. Physical Review Research, 2020, 2, .	3.6	12
8	Many-body perturbation theory calculations using the yambo code. Journal of Physics Condensed Matter, 2019, 31, 325902.	1.8	269
9	Engineering the Interfacial Electronic Structure of Epitaxial Ge/AlAs(001) Heterointerfaces via Substitutional Boron Incorporation: The Roles of Doping and Interface Stoichiometry. ACS Applied Electronic Materials, 2019, 1, 2646-2654.	4.3	7
10	Possible phonon-induced electronic bi-stability in VO2 for ultrafast memory at room temperature. , 2019, , .		1
11	Second-harmonic generation in single-layer monochalcogenides: A response from first-principles real-time simulations. Physical Review Materials, 2019, 3, .	2.4	23
12	Spectroscopic Size and Thickness Metrics for Liquid-Exfoliated h-BN. Chemistry of Materials, 2018, 30, 1998-2005.	6.7	65
13	Satellite valleys and strained band gap transition of bulk Ge: Impact of pseudopotential approximations on quasiparticle levels. Computational Materials Science, 2018, 149, 115-124.	3.0	1
14	First-Principles Calculations of Band Offsets at Heterovalent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Îµ</mml:mi></mml:math> - <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Ge</mml:mi><mml:mi>In</mml:mi></mml:mrow><mml:mi>x</mml:mi></mml:m Physical Review Applied, 2018, 10, .	3.8	3
15	Two-photon absorption in two-dimensional materials: The case of hexagonal boron nitride. Physical Review B, 2018, 98, .	3.2	22
16	Direct and indirect band gaps in Ge under biaxial tensile strain investigated by photoluminescence and photoreflectance studies. Physical Review B, 2018, 97, .	3.2	18
17	Second-Harmonic Generation in Two-Dimensional Materials. , 2018, , 284-290.		0
18	Effect of ladder diagrams on optical absorption spectra in a quasiparticle self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="italic">GW</mml:mi></mml:math> framework. Physical Review Materials, 2018, 2, .	2.4	45

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19	Excitonic effects in third-harmonic generation: The case of carbon nanotubes and nanoribbons. Physical Review B, 2017, 95, .	3.2	27
20	Optical properties of periodic systems within the current-current response framework: Pitfalls and remedies. Physical Review B, 2017, 95, .	3.2	22
21	Performance of polarisation functionals for linear and nonlinear optical properties of bulk zinc chalcogenides ZnX (X = S, Se, and Te). Physical Chemistry Chemical Physics, 2016, 18, 21179-21189.	2.8	13
22	Projected equations of motion approach to hybrid quantum/classical dynamics in dielectric-metal composites. Physical Review B, 2016, 94, .	3.2	8
23	Dielectrics in a time-dependent electric field: A real-time approach based on density-polarization functional theory. Physical Review B, 2016, 94, .	3.2	20
24	Strong second harmonic generation in SiC, ZnO, GaN two-dimensional hexagonal crystals from first-principles many-body calculations. Physical Chemistry Chemical Physics, 2015, 17, 9533-9540.	2.8	47
25	Second harmonic generation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>h</mml:mi></mml:math>-BN and MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>monolayers: Role of electron-hole interaction. Physical Review B, 2014, 89, .	3.2	97
26	Nonlinear optics from anab initioapproach by means of the dynamical Berry phase: Application to second- and third-harmonic generation in semiconductors. Physical Review B, 2013, 88, .	3.2	62
27	Time-dependent density functional theory study of charge transfer in collisions. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	21
28	Implementation and testing of Lanczos-based algorithms for Random-Phase Approximation eigenproblems. Computational Materials Science, 2011, 50, 2148-2156.	3.0	37
29	Electronic properties of interfaces and defects from manyâ€body perturbation theory: Recent developments and applications. Physica Status Solidi (B): Basic Research, 2011, 248, 275-289.	1.5	91
30	Real-time approach to the optical properties of solids and nanostructures: Time-dependent Bethe-Salpeter equation. Physical Review B, 2011, 84, .	3.2	103
31	Local-field and excitonic effects in the optical response of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi></mml:mrow></mml:math>-alumina. Physical Review B, 2011, 83, .	3.2	12
32	Quasiparticle calculations of the electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>HfO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>and their interface with Si. Physical Review B, 2010, 81, .	3.2	35
33	Electronic properties of zircon and hafnon from many-body perturbation theory. Physical Review B, 2009, 79, .	3.2	12
34	yambo: An ab initio tool for excited state calculations. Computer Physics Communications, 2009, 180, 1392-1403.	7.5	927
35	Exciton-Plasmon States in Nanoscale Materials: Breakdown of the Tammâ€“Dancoff Approximation. Nano Letters, 2009, 9, 2820-2824.	9.1	128
36	Comment on â€œHuge Excitonic Effects in Layered Hexagonal Boron Nitrideâ€• Physical Review Letters, 2008, 100, 189701; discussion 189702.	7.8	64

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37	Macroscopic limit of time-dependent density-functional theory for adiabatic local approximations of the exchange-correlation kernel. Physical Review B, 2007, 76, .	3.2	7
38	Density functionals from many-body perturbation theory: The band gap for semiconductors and insulators. Journal of Chemical Physics, 2006, 124, 154108.	3.0	166
39	Effect of spatial nonlocality on the density functional band gap. Physical Review B, 2006, 74, .	3.2	68
40	Performance of Density Functionals for Calculating Barrier Heights of Chemical Reactions Relevant to Astrophysics. Journal of Physical Chemistry A, 2004, 108, 7621-7636.	2.5	80
41	Improved Description of Chemical Barriers with Generalized Gradient Approximations (GGAs) and Meta-GGAs. Journal of Physical Chemistry A, 2004, 108, 4459-4469.	2.5	48
42	STO and GTO field-induced polarization functions for H to Kr. Journal of Computational Chemistry, 2003, 24, 1582-1591.	3.3	21
43	Exchange-correlation energy and potential as approximate functionals of occupied and virtual Kohnâ€“Sham orbitals: Application to dissociating H[sub 2]. Journal of Chemical Physics, 2003, 118, 7183.	3.0	54
44	On the required shape corrections to the local density and generalized gradient approximations to the Kohnâ€“Sham potentials for molecular response calculations of (hyper)polarizabilities and excitation energies. Journal of Chemical Physics, 2002, 116, 9591-9601.	3.0	113
45	Exchange potential from the common energy denominator approximation for the Kohnâ€“Sham Greenâ€™s function: Application to (hyper)polarizabilities of molecular chains. Journal of Chemical Physics, 2002, 116, 6435-6442.	3.0	91
46	Shape corrections to exchange-correlation potentials by gradient-regulated seamless connection of model potentials for inner and outer region. Journal of Chemical Physics, 2001, 114, 652.	3.0	343
47	The Failure of Generalized Gradient Approximations (GGAs) and Meta-GGAs for the Two-Center Three-Electron Bonds in He2+, (H2O)2+, and (NH3)2+. Journal of Physical Chemistry A, 2001, 105, 9211-9218.	2.5	83
48	Density Functional Study of the Photoactive Yellow Protein's Chromophore. Journal of Physical Chemistry B, 2001, 105, 4386-4391.	2.6	59