# Myrta GrÃ¼ning

## List of Publications by Year
in descending order

| 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 | yambo: An ab initio tool for excited state calculations. Computer Physics Communications, 2009, 180, 1392-1403. | 7.5 | 927 |
| 2 | 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 |
| 3 | Many-body perturbation theory calculations using the yambo code. Journal of Physics Condensed Matter, 2019, 31, 325902. | 1.8 | 269 |
| 4 | Density functionals from many-body perturbation theory: The band gap for semiconductors and insulators. Journal of Chemical Physics, 2006, 124, 154108. | 3.0 | 166 |
| 5 | Exciton-Plasmon States in Nanoscale Materials: Breakdown of the Tamm‒Dancoff Approximation. Nano Letters, 2009, 9, 2820-2824. | 9.1 | 128 |
| 6 | On the required shape corrections to the local density and generalized gradient approximations to the Kohn–Sham potentials for molecular response calculations of (hyper)polarizabilities and excitation energies. Journal of Chemical Physics, 2002, 116, 9591-9601. | 3.0 | 113 |
| 7 | Real-time approach to the optical properties of solids and nanostructures: Time-dependent Bethe-Salpeter equation. Physical Review B, 2011, 84, . | 3.2 | 103 |
| 8 | Second harmonic generation in $h$-BN and $MoS_2$ monolayers: Role of electron-hole interaction. Physical Review B, 2014, 89, . | 3.2 | 97 |
| 9 | Exchange potential from the common energy denominator approximation for the Kohn–Sham Green's function: Application to (hyper)polarizabilities of molecular chains. Journal of Chemical Physics, 2002, 116, 6435-6442. | 3.0 | 91 |
| 10 | Electronic properties of interfaces and defects from many‐body perturbation theory: Recent developments and applications. Physica Status Solidi (B): Basic Research, 2011, 248, 275-289. | 1.5 | 91 |
| 11 | 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 |
| 12 | 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 |
| 13 | Effect of spatial nonlocality on the density functional band gap. Physical Review B, 2006, 74, . | 3.2 | 68 |
| 14 | Spectroscopic Size and Thickness Metrics for Liquid-Exfoliated $h$-BN. Chemistry of Materials, 2018, 30, 1998-2005. | 6.7 | 65 |
| 15 | Comment on "Huge Excitonic Effects in Layered Hexagonal Boron Nitride". Physical Review Letters, 2008, 100, 189701; discussion 189702. | 7.8 | 64 |
| 16 | Nonlinear optics from an *ab initio* approach by means of the dynamical Berry phase: Application to second- and third-harmonic generation in semiconductors. Physical Review B, 2013, 88, . | 3.2 | 62 |
| 17 | Density Functional Study of the Photoactive Yellow Protein's Chromophore. Journal of Physical Chemistry B, 2001, 105, 4386-4391. | 2.6 | 59 |
| 18 | Exchange-correlation energy and potential as approximate functionals of occupied and virtual Kohn–Sham orbitals: Application to dissociating H[sub 2]. Journal of Chemical Physics, 2003, 118, 7183. | 3.0 | 54 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Effect of ladder diagrams on optical absorption spectra in a quasiparticle self-consistent $GW$ framework. Physical Review Materials, 2018, 2, . | 2.4 | 45 |
| 22 | Implementation and testing of Lanczos-based algorithms for Random-Phase Approximation eigenproblems. Computational Materials Science, 2011, 50, 2148-2156. | 3.0 | 37 |
| 23 | Quasiparticle calculations of the electronic properties of $ZrO_2$ and $HfO_2$ and their interface with Si. Physical Review B, 2010, 81, . | 3.2 | 35 |
| 24 | Excitonic effects in third-harmonic generation: The case of carbon nanotubes and nanoribbons. Physical Review B, 2017, 95, . | 3.2 | 27 |
| 25 | Second-harmonic generation in single-layer monochalcogenides: A response from first-principles real-time simulations. Physical Review Materials, 2019, 3, . | 2.4 | 23 |
| 26 | Optical properties of periodic systems within the current-current response framework: Pitfalls and remedies. Physical Review B, 2017, 95, . | 3.2 | 22 |
| 27 | Two-photon absorption in two-dimensional materials: The case of hexagonal boron nitride. Physical Review B, 2018, 98, . | 3.2 | 22 |
| 28 | STO and GTO field-induced polarization functions for H to Kr. Journal of Computational Chemistry, 2003, 24, 1582-1591. | 3.3 | 21 |
| 29 | Time-dependent density functional theory study of charge transfer in collisions. Theoretical Chemistry Accounts, 2012, 131, 1. | 1.4 | 21 |
| 30 | 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 |
| 31 | 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 |
| 32 | Optical response and band structure of $LiCoO_2$ including electron-hole interaction effects. Physical Review B, 2021, 104, . | 3.2 | 18 |
| 33 | Electronic structure of chromium trihalides beyond density functional theory. Physical Review B, 2021, 104, . | 3.2 | 18 |
| 34 | 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 |
| 35 | Electronic properties of zircon and hafnon from many-body perturbation theory. Physical Review B, 2009, 79, . | 3.2 | 12 |
| 36 | Local-field and excitonic effects in the optical response of $\alpha$-alumina. Physical Review B, 2011, 83, . | 3.2 | 12 |

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|---|---------|----|-----------| 
| 37 | `<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 |
| 38 | Towards temperature-induced topological phase transition in SnTe: A first-principles study. Physical Review B, 2020, 101, . | 3.2 | 9 |
| 39 | Role of the lattice in the light-induced insulator-to-metal transition in vanadium dioxide. Physical Review Research, 2020, 2, . | 3.6 | 9 |
| 40 | Projected equations of motion approach to hybrid quantum/classical dynamics in dielectric-metal composites. Physical Review B, 2016, 94, . | 3.2 | 8 |
| 41 | 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 |
| 42 | 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 |
| 43 | Electronic Materials, 2019, 1, 2646-2654. Band Offsets at Heterovalent `<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Î¼</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:msub></mml:math>` Physical Review Applied, 2018, 10, . | 3.8 | 3 |
| 44 | Double k-Grid Method for Solving the Bethe-Salpeter Equation via Lanczos Approaches. Frontiers in Chemistry, 2021, 9, 763946. | 3.6 | 2 |
| 45 | 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 |
| 46 | Possible phonon-induced electronic bi-stability in VO2 for ultrafast memory at room temperature. , 2019, , . | | 1 |
| 47 | Second-Harmonic Generation in Two-Dimensional Materials. , 2018, , 284-290. | | 0 |
| 48 | Thermal conductivity of porous polycrystalline PbTe. Physical Review Materials, 2021, 5, . | 2.4 | 0 |