# Xinguo Ren

List of Publications by Year
in descending order

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| 63 | 6,066 | 172386 | 118793 |
|---|---|---|---|
| papers | citations | 29 | 62 |
| | | h-index | g-index |

| 64 | 64 | 64 | 5062 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Ab initio molecular simulations with numeric atom-centered orbitals. Computer Physics Communications, 2009, 180, 2175-2196. | 3.0 | 2,170 |
| 2 | Resolution-of-identity approach to Hartreeâ€“Fock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. New Journal of Physics, 2012, 14, 053020. | 1.2 | 549 |
| 3 | Random-phase approximation and its applications in computational chemistry and materials science. Journal of Materials Science, 2012, 47, 7447-7471. | 1.7 | 479 |
| 4 | GW100: Benchmarking G<sub>0</sub>W<sub>0</sub> for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687. | 2.3 | 280 |
| 5 | Beyond the Random-Phase Approximation for the Electron Correlation Energy: The Importance of Single Excitations. Physical Review Letters, 2011, 106, 153003. | 2.9 | 193 |
| 6 | Benchmark of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>methods for azabenzenes. Physical Review B, 2012, 86, . | 1.1 | 154 |
| 7 | Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods. Journal of Chemical Theory and Computation, 2016, 12, 615-626. | 2.3 | 154 |
| 8 | Exploring the random phase approximation: Application to CO adsorbed on Cu(111). Physical Review B, 2009, 80, . | 1.1 | 147 |
| 9 | Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. New Journal of Physics, 2013, 15, 053046. | 1.2 | 143 |
| 10 | Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002. | 1.2 | 137 |
| 11 | Self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>: All-electron implementation with localized basis functions. Physical Review B, 2013, 88, . | 1.1 | 135 |
| 12 | Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. Computer Physics Communications, 2015, 192, 60-69. | 3.0 | 133 |
| 13 | Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. Physical Review B, 2013, 88, . | 1.1 | 113 |
| 14 | Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. New Journal of Physics, 2015, 17, 093020. | 1.2 | 97 |
| 15 | Electronic structure of copper phthalocyanine from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub><mml:msub><mml:mi>W</mml:mi> Physical Review B, 2011, 84, . | 1.1 | 86 |
| 16 | Bond Breaking and Bond Formation: How Electron Correlation is Captured in Many-Body Perturbation Theory and Density-Functional Theory. Physical Review Letters, 2013, 110, 146403. | 2.9 | 82 |
| 17 | Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. New Journal of Physics, 2013, 15, 123033. | 1.2 | 81 |
| 18 | Real-time GW -BSE investigations on spin-valley exciton dynamics in monolayer transition metal dichalcogenide. Science Advances, 2021, 7, . | 4.7 | 70 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Density-Functional Theory for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>f</mml:mi></mml:math>-Electron Systems: The<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:mi>Î³</mml:mi></mml:math>Phase Transition in Cerium. Physical Review Letters, 2012, 109, 146402. | 2.9 | 62 |
| 20 | Large-scale ab initio simulations based on systematically improvable atomic basis. Computational Materials Science, 2016, 112, 503-517. | 1.4 | 61 |
| 21 | Static correlation and electron localization in molecular dimers from the self-consistent RPA and<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:m Physical Review B, 2015, 91, . | 1.1 | 54 |
| 22 | Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. Physical Review B, 2016, 94, . | 1.1 | 52 |
| 23 | Beyond the<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:m A second-order screened exchange correction. Physical Review B, 2015, 92, . | 1.1 | 49 |
| 24 | First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory. Physical Review B, 2014, 90, . | 1.1 | 44 |
| 25 | Electronic structure of dye-sensitized TiO<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>clusters from many-body perturbation theory. Physical Review B, 2011, 84, . | 1.1 | 41 |
| 26 | All-electron ab initio Bethe-Salpeter equation approach to neutral excitations in molecules with numeric atom-centered orbitals. Journal of Chemical Physics, 2020, 152, 044105. | 1.2 | 38 |
| 27 | High-Resolution Model for Noncontact Atomic Force Microscopy with a Flexible Molecule on the Tip Apex. Journal of Physical Chemistry C, 2015, 119, 1483-1488. | 1.5 | 34 |
| 28 | Self-consistent Green's function embedding for advanced electronic structure methods based on a dynamical mean-field concept. Physical Review B, 2016, 93, . | 1.1 | 34 |
| 29 | Toward Low-Temperature Dehydrogenation Catalysis: Isophorone Adsorbed on Pd(111). Journal of Physical Chemistry Letters, 2012, 3, 582-586. | 2.1 | 33 |
| 30 | Size Effects in the Interface Level Alignment of Dye-Sensitized TiO<sub>2</sub> Clusters. Journal of Physical Chemistry Letters, 2014, 5, 2395-2401. | 2.1 | 28 |
| 31 | Origin of the Contrast Interpreted as Intermolecular and Intramolecular Bonds in Atomic Force Microscopy Images. Journal of Physical Chemistry C, 2015, 119, 14195-14200. | 1.5 | 27 |
| 32 | All-electron periodic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:m implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. Physical Review Materials, 2021, 5, . | 0.9 | 25 |
| 33 | Density functional theory study of theÎ±â^'Î³phase transition in cerium: Role of electron correlation andf-orbital localization. Physical Review B, 2016, 93, . | 1.1 | 23 |
| 34 | The origin of hyperferroelectricity in LiBO3 (Bâ€‰=â€‰V, Nb, Ta, Os). Scientific Reports, 2016, 6, 34085. | 1.6 | 21 |
| 35 | On the room-temperature phase diagram of high pressure hydrogen: An ab initio molecular dynamics perspective and a diffusion Monte Carlo study. Journal of Chemical Physics, 2014, 141, 024501. | 1.2 | 19 |
| 36 | Accuracy of Localized Resolution of the Identity in Periodic Hybrid Functional Calculations with Numerical Atomic Orbitals. Journal of Physical Chemistry Letters, 2020, 11, 3082-3088. | 2.1 | 17 |

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|---|---|---|---|
| 37 | Directional Growth of One-Dimensional CO<sub>2</sub> Chains on ZnO(101Ì…0). Journal of Physical Chemistry C, 2016, 120, 23669-23674. | 1.5 | 16 |
| 38 | Cooperative Effect in a Graphite Intercalation Compound: Enhanced Mobility of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Al</mml:mi><mml:mi>Cl</mml:mi></mml:mrow><mml:mn>4</mml:mn></mml:r in the Graphite Cathode of Aluminum-Ion Batteries. Physical Review Applied, 2019, 12, . | 1.5 | 15 |
| 39 | Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: systematic benchmark of the numerical and intrinsic errors in state-of-the-art electronic-structure approximations. New Journal of Physics, 2019, 21, 013025. | 1.2 | 15 |
| 40 | Assessing the G<sub>0</sub>W<sub>0</sub>Î“<sub>0</sub><sup>(1)</sup> Approach: Beyond G<sub>0</sub>W<sub>0</sub> with Hedinâ€™s Full Second-Order Self-Energy Contribution. Journal of Chemical Theory and Computation, 2021, 17, 5140-5154. | 2.3 | 13 |
| 41 | First-principles calculations and model analysis of plasmon excitations in graphene and graphene/hBN heterostructure. Physical Review B, 2017, 96, . | 1.1 | 12 |
| 42 | A DFT study of energetic and structural properties of a full turn of A-form DNA under relaxed and stretching conditions. Journal of Chemical Physics, 2019, 151, 215102. | 1.2 | 12 |
| 43 | Efficient Hybrid Density Functional Calculations for Large Periodic Systems Using Numerical Atomic Orbitals. Journal of Chemical Theory and Computation, 2021, 17, 222-239. | 2.3 | 12 |
| 44 | First-principles molecular dynamics study of deuterium diffusion in liquid tin. Journal of Chemical Physics, 2017, 147, 064505. | 1.2 | 11 |
| 45 | Identifying Different Adsorption States of Methanol on ZnO(101Ì…0): A Scanning Tunneling Microscopy and Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 9105-9111. | 1.5 | 9 |
| 46 | Metal adatoms generated by the co-play of melamine assembly and subsequent CO adsorption. Physical Chemistry Chemical Physics, 2016, 18, 2324-2329. | 1.3 | 8 |
| 47 | First-principles calculation of optical responses based on nonorthogonal localized orbitals. New Journal of Physics, 2019, 21, 093001. | 1.2 | 8 |
| 48 | Comparing particle-particle and particle-hole channels of the random phase approximation. Physical Review B, 2019, 99, . | 1.1 | 8 |
| 49 | Beryllium and Magnesium Metal Clusters: New Globally Stable Structures and G0W0 Calculations. Journal of Physical Chemistry A, 2021, 125, 1424-1435. | 1.1 | 8 |
| 50 | First-principles study of the electronic and optical properties of Li(Nb,Os)O3 alloys. Applied Physics Letters, 2018, 112, . | 1.5 | 7 |
| 51 | Strategy for constructing compact numerical atomic orbital basis sets by incorporating the gradients of reference wavefunctions. Physical Review B, 2021, 103, . | 1.1 | 7 |
| 52 | Intercalation of van der Waals layered materials: A route towards engineering of electron correlation*. Chinese Physics B, 2020, 29, 097104. | 0.7 | 7 |
| 53 | Strong charge and spin fluctuations inLa2O3Fe2Se2. Physical Review B, 2016, 94, . | 1.1 | 6 |
| 54 | Real-Time, Time-Dependent Density Functional Theory Study on Photoinduced Isomerizations of Azobenzene Under a Light Field. Journal of Physical Chemistry Letters, 2022, 13, 427-432. | 2.1 | 6 |

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|---|---|---|---|
| 55 | Exploring Molecules beyond CO as Tip Functionalizations in High-Resolution Noncontact Atomic Force Microscopy: A First Principles Approach. ACS Omega, 2016, 1, 1004-1009. | 1.6 | 4 |
| 56 | Phase stability of the argon crystal: first-principles study based on random phase approximation plus renormalized single excitation corrections. New Journal of Physics, 2022, 24, 033049. | 1.2 | 4 |
| 57 | DFT+U within the framework of linear combination of numerical atomic orbitals. Journal of Chemical Physics, 2022, 156, . | 1.2 | 4 |
| 58 | Retention and recycling of deuterium in liquid lithium-tin slab studied by first-principles molecular dynamics. Journal of Nuclear Materials, 2021, 543, 152542. | 1.3 | 2 |
| 59 | Self-Interaction-Corrected Random Phase Approximation. Journal of Chemical Theory and Computation, 2021, 17, 2107-2115. | 2.3 | 2 |
| 60 | Accurate stress calculations based on numerical atomic orbital bases: Implementation and benchmarks. Computer Physics Communications, 2021, 267, 108043. | 3.0 | 2 |
| 61 | Long-range behavior of a nonlocal correlation-energy density functional based on the random-phase approximation. Physical Review B, 2020, 101, . | 1.1 | 1 |
| 62 | First-principles study of benzo[a]pyrene-7,8-dione and DNA adducts. Journal of Chemical Physics, 2021, 154, 175102. | 1.2 | 1 |
| 63 | Peculiar diffusion behavior of AlCl4 intercalated in graphite from nanosecond-long molecular dynamics simulations. Chinese Physics B, 0, , . | 0.7 | 1 |