# Peilin Liao

## List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/4079407/publications.pdf

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|---|---|---|---|
| 45 papers | 4,856 citations | 218381 26 h-index | 233125 45 g-index |
| 47 all docs | 47 docs citations | 47 times ranked | 7282 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Destruction of chemical warfare agents using metalâ€“organic frameworks. Nature Materials, 2015, 14, 512-516. | 13.3 | 790 |
| 2 | Water Oxidation on Pure and Doped Hematite (0001) Surfaces: Prediction of Co and Ni as Effective Dopants for Electrocatalysis. Journal of the American Chemical Society, 2012, 134, 13296-13309. | 6.6 | 492 |
| 3 | Interfacing nickel nitride and nickel boosts both electrocatalytic hydrogen evolution and oxidation reactions. Nature Communications, 2018, 9, 4531. | 5.8 | 410 |
| 4 | First principles scheme to evaluate band edge positions in potential transition metal oxide photocatalysts and photoelectrodes. Physical Chemistry Chemical Physics, 2011, 13, 16644. | 1.3 | 380 |
| 5 | Molecular engineering of organicâ€“inorganic hybrid perovskites quantum wells. Nature Chemistry, 2019, 11, 1151-1157. | 6.6 | 302 |
| 6 | Rotationally invariant ab initio evaluation of Coulomb and exchange parameters for DFT+U calculations. Journal of Chemical Physics, 2008, 129, 014103. | 1.2 | 282 |
| 7 | Electron Transport in Pure and Doped Hematite. Nano Letters, 2011, 11, 1775-1781. | 4.5 | 267 |
| 8 | New concepts and modeling strategies to design and evaluate photo-electro-catalysts based on transition metal oxides. Chemical Society Reviews, 2013, 42, 2401-2422. | 18.7 | 225 |
| 9 | Highly Stable Lead-Free Perovskite Field-Effect Transistors Incorporating Linear Ï€-Conjugated Organic Ligands. Journal of the American Chemical Society, 2019, 141, 15577-15585. | 6.6 | 180 |
| 10 | Distribution and Valence State of Ru Species on CeO<sub>2</sub> Supports: Support Shape Effect and Its Influence on CO Oxidation. ACS Catalysis, 2019, 9, 11088-11103. | 5.5 | 159 |
| 11 | Testing variations of the GW approximation on strongly correlated transition metal oxides: hematite (Î±-Fe2O3) as a benchmark. Physical Chemistry Chemical Physics, 2011, 13, 15189. | 1.3 | 135 |
| 12 | Interfacial Sites between Cobalt Nitride and Cobalt Act as Bifunctional Catalysts for Hydrogen Electrochemistry. ACS Energy Letters, 2019, 4, 1594-1601. | 8.8 | 128 |
| 13 | Origin of the Energy Barrier to Chemical Reactions of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>on Al(111): Evidence for Charge Transfer, Not Spin Selection. Physical Review Letters, 2012, 109, 198303. | 2.9 | 125 |
| 14 | Titanium incorporation into hematite photoelectrodes: theoretical considerations and experimental observations. Energy and Environmental Science, 2014, 7, 3100-3121. | 15.6 | 118 |
| 15 | Layer-by-layer anionic diffusion in two-dimensional halide perovskite vertical heterostructures. Nature Nanotechnology, 2021, 16, 584-591. | 15.6 | 88 |
| 16 | Hole transport in pure and doped hematite. Journal of Applied Physics, 2012, 112, . | 1.1 | 84 |
| 17 | A Surfaceâ€Oxideâ€Rich Activation Layer (SOAL) on Ni<sub>2</sub>Mo<sub>3</sub>N for a Rapid and Durable Oxygen Evolution Reaction. Angewandte Chemie - International Edition, 2020, 59, 18036-18041. | 7.2 | 77 |
| 18 | Optical Excitations in Hematite (Î±-Fe<sub>2</sub>O<sub>3</sub>) via Embedded Cluster Models: A CASPT2 Study. Journal of Physical Chemistry C, 2011, 115, 20795-20805. | 1.5 | 57 |

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|---|---|---|---|
| 19 | Insights into Catalytic Hydrolysis of Organophosphate Warfare Agents by Metalâ€“Organic Framework NU-1000. Journal of Physical Chemistry C, 2018, 122, 12362-12368. | 1.5 | 55 |
| 20 | Ligand-Driven Grain Engineering of High Mobility Two-Dimensional Perovskite Thin-Film Transistors. Journal of the American Chemical Society, 2021, 143, 15215-15223. | 6.6 | 55 |
| 21 | Ab initio DFT + U predictions of tensile properties of iron oxides. Journal of Materials Chemistry, 2010, 20, 6703. | 6.7 | 45 |
| 22 | Optimizing Open Iron Sites in Metalâ€“Organic Frameworks for Ethane Oxidation: A First-Principles Study. ACS Applied Materials & Interfaces, 2017, 9, 33484-33492. | 4.0 | 44 |
| 23 | Strainâ€Engineered Anisotropic Optical and Electrical Properties in 2D Chiralâ€Chain Tellurium. Advanced Materials, 2020, 32, e2002342. | 11.1 | 40 |
| 24 | Neural network reactive force field for C, H, N, and O systems. Npj Computational Materials, 2021, 7, . | 3.5 | 39 |
| 25 | Alkaline-earth metal-oxide overlayers on TiO<sub>2</sub>: application toward CO<sub>2</sub> photoreduction. Catalysis Science and Technology, 2016, 6, 7885-7895. | 2.1 | 29 |
| 26 | Steering Onâ€Surface Reactions by a Selfâ€Assembly Approach. Angewandte Chemie - International Edition, 2017, 56, 5026-5030. | 7.2 | 28 |
| 27 | Metal-to-insulator transition in SmNiO<sub>3</sub> induced by chemical doping: a first principles study. Molecular Systems Design and Engineering, 2018, 3, 264-274. | 1.7 | 24 |
| 28 | First principles study on hydrogen doping induced metal-to-insulator transition in rare earth nickelates RNiO<sub>3</sub> (R = Pr, Nd, Sm, Eu, Gd, Tb, Dy, Yb). Physical Chemistry Chemical Physics, 2020, 22, 6888-6895. | 1.3 | 23 |
| 29 | Low-temperature scanning tunneling microscopy study on the electronic properties of a double-decker DyPc2 molecule at the surface. Physical Chemistry Chemical Physics, 2015, 17, 27019-27026. | 1.3 | 22 |
| 30 | Molecular Building Block-Based Electronic Charges for High-Throughput Screening of Metalâ€“Organic Frameworks for Adsorption Applications. Journal of Chemical Theory and Computation, 2018, 14, 365-376. | 2.3 | 18 |
| 31 | Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. Catalysis Today, 2018, 312, 149-157. | 2.2 | 16 |
| 32 | Detection and Manipulation of Charge States for Double-Decker DyPc<sub>2</sub> Molecules on Ultrathin CuO Films. ACS Nano, 2018, 12, 2991-2997. | 7.3 | 16 |
| 33 | Steering the Achiral into Chiral with a Self-Assembly Strategy. ACS Nano, 2019, 13, 7202-7208. | 7.3 | 16 |
| 34 | Stabilizing surface Ag adatoms into tunable single atom arrays by terminal alkyne assembly. Chemical Communications, 2016, 52, 12944-12947. | 2.2 | 15 |
| 35 | Steering Onâ€Surface Reactions by a Selfâ€Assembly Approach. Angewandte Chemie, 2017, 129, 5108-5112. | 1.6 | 14 |
| 36 | Ab initio density functional theory+U predictions of the shear response of iron oxides. Acta Materialia, 2010, 58, 5912-5925. | 3.8 | 11 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | A computational study of hydrogen doping induced metal-to-insulator transition in CaFeO<sub>3</sub>, SrFeO<sub>3</sub>, BaFeO<sub>3</sub> and SmMnO<sub>3</sub>. Physical Chemistry Chemical Physics, 2019, 21, 25397-25405. | 1.3 | 8 |
| 38 | Parallel Nanoimprint Forming of One-Dimensional Chiral Semiconductor for Strain-Engineered Optical Properties. Nano-Micro Letters, 2020, 12, 160. | 14.4 | 8 |
| 39 | Catalytic Light Alkanes Conversion through Anaerobic Ammodehydrogenation. ACS Catalysis, 2021, 11, 7987-7995. | 5.5 | 8 |
| 40 | Facile Synthesis of Pt Carbide Nanomaterials and Their Catalytic Applications. , 2021, 3, 179-186. | | 8 |
| 41 | Chiral features of metal phthalocyanines sitting atop the pre-assembled TiOPc monolayer on Ag(111). Physical Chemistry Chemical Physics, 2019, 21, 16323-16328. | 1.3 | 5 |
| 42 | A Surfaceâ€Oxideâ€Rich Activation Layer (SOAL) on Ni 2 Mo 3 N for a Rapid and Durable Oxygen Evolution Reaction. Angewandte Chemie, 2020, 132, 18192-18197. | 1.6 | 4 |
| 43 | Structural Tunability and Diversity of Twoâ€Dimensional Lead Halide Benzenethiolate. Chemistry - A European Journal, 2020, 26, 6599-6607. | 1.7 | 3 |
| 44 | Online simulation powered learning modules for materials science. MRS Advances, 2019, 4, 2727-2742. | 0.5 | 1 |
| 45 | Doping-Enabled Reconfigurable Strongly Correlated Phase in a Quasi-2D Perovskite. Journal of Physical Chemistry Letters, 2021, 12, 5091-5098. | 2.1 | 1 |