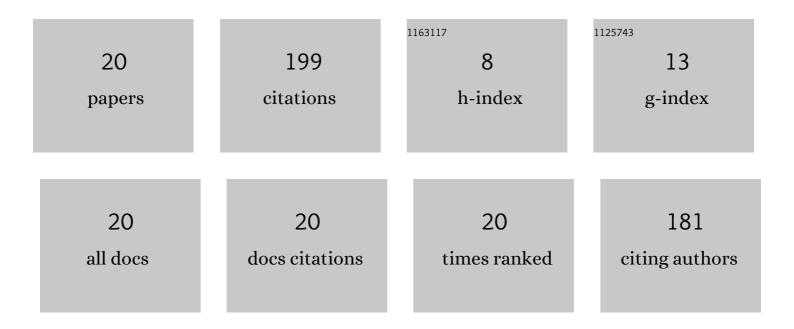


List of Publications by Year in descending order

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| # | Article | IF | CITATIONS |
|----|--|------|-----------|
| 1 | Exploring Highly Efficient Dual-Metal-Site Electrocatalysts for Oxygen Reduction Reaction by First Principles Screening. Journal of the Electrochemical Society, 2022, 169, 026524. | 2.9 | 9 |
| 2 | Computational evaluation of ScB and TiB MBenes as promising anode materials for high-performance metal-ion batteries. Physical Review Materials, 2022, 6, . | 2.4 | 4 |
| 3 | Computational screening of MBene monolayers with high electrocatalytic activity for the nitrogen reduction reaction. Nanoscale, 2021, 13, 15002-15009. | 5.6 | 22 |
| 4 | Oxygen adsorption on high-index faceted Pt nanoparticles. Physical Chemistry Chemical Physics, 2021, 23, 17323-17328. | 2.8 | 4 |
| 5 | Structural Evolution of the Surface and Interface in Bimetallic High-Index Faceted Heterogeneous Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 2454-2462. | 4.6 | 5 |
| 6 | Single Mn Atom Anchored on Nitrogenâ€Doped Graphene as a Highly Efficient Electrocatalyst for Oxygen Reduction Reaction. Chemistry - A European Journal, 2021, 27, 9686-9693. | 3.3 | 15 |
| 7 | Molecular Dynamics Simulations of Thermally Induced Surface and Shape Evolution of Concave Au Nanocubes: Implications for Catalysis. ACS Applied Nano Materials, 2021, 4, 9527-9535. | 5.0 | 2 |
| 8 | Boosting the Electrocatalytic Activity of Feâ^'Co Dualâ€Atom Catalysts for Oxygen Reduction Reaction by Ligandâ€Modification Engineering. ChemCatChem, 2021, 13, 4645-4651. | 3.7 | 11 |
| 9 | Computational screening of pristine and functionalized ordered TiVC MXenes as highly efficient anode materials for lithium-ion batteries. Nanoscale, 2021, 13, 2995-3001. | 5.6 | 22 |
| 10 | Computational screening of efficient graphene-supported transition metal single atom catalysts toward the oxygen reduction reaction. Journal of Materials Chemistry A, 2020, 8, 19319-19327. | 10.3 | 49 |
| 11 | Basin Hopping Genetic Algorithm for Global Optimization of PtCo Clusters. Journal of Chemical Information and Modeling, 2020, 60, 2219-2228. | 5.4 | 12 |
| 12 | Structural, magnetic, and electronic properties of small M-Pt (MÂ=ÂFe, Co, and Ni) clusters: Insight from density-functional calculations. Journal of Magnetism and Magnetic Materials, 2020, 512, 167047. | 2.3 | 4 |
| 13 | Thermal Stability of Unary to Quinary Noble-Metal/3d-Transition-Metal Alloy Nanoparticles from Molecular Dynamics Simulations: Implications for Multimetallic Catalysis. ACS Applied Nano Materials, 2020, 3, 5381-5389. | 5.0 | 9 |
| 14 | Structural and magnetic properties of Co-Pt clusters: A spin-polarized density functional study. Journal of Magnetism and Magnetic Materials, 2020, 503, 166651. | 2.3 | 3 |
| 15 | Solid–Liquid Coexistence in Trimetallic Heterostructured Nanoparticle Catalysts: Insights from Molecular Dynamics Simulations. ACS Applied Nano Materials, 2020, 3, 12369-12378. | 5.0 | 10 |
| 16 | [2+1] Additions of (n,0)(n=6â^'10) single-walled carbon nanotubes with di-vacancies based on defect curvature: A first-principles study. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950004. | 1.8 | 1 |
| 17 | Structural Transformation and Cycling Improvement of Nanosized Flower-like Î ³ -MnO ₂ in a Sodium Battery. ACS Applied Energy Materials, 2019, 2, 5050-5056. | 5.1 | 13 |
| 18 | [1+1] and [2+1] Additions on a (5,5) Single-Walled Carbon Nanotube with V ₁ ~V ₄ Vacancies Based on Defect Curvature: A First Principles Study. Acta Chimica Sinica, 2017, 75, 284. | 1.4 | 1 |

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|----|---|-----|-----------|
| 19 | Curvature, vacancy size and chirality effects of mono- to octa-vacancies in zigzag single-walled carbon nanotubes. New Journal of Chemistry, 2016, 40, 8625-8631. | 2.8 | 1 |
| 20 | Molecular Dynamics Investigation on Thermal Stability and Shape Evolution of Pd-Au Heterostructured Nanorods: Implications for Catalysis. ACS Applied Nano Materials, 0, , . | 5.0 | 2 |