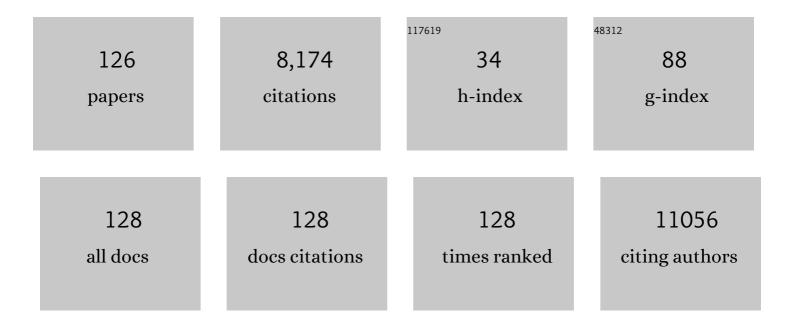
List of Publications by Year in descending order

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| # | Article | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Following the light: 3D-printed COF@poly(2-hydroxyethyl methacrylate) dual emissive composite with response to polarity and acidity. Journal of Materials Chemistry A, 2022, 10, 4634-4643. | 10.3 | 15 |
| 2 | Pyrenetetraone-based covalent organic framework as an effective electrocatalyst for oxygen reduction reaction. Nano Research, 2022, 15, 3907-3912. | 10.4 | 14 |
| 3 | Covalent organic frameworks based on electroactive naphthalenediimide as active electrocatalysts toward oxygen reduction reaction. Applied Materials Today, 2022, 26, 101384. | 4.3 | 13 |
| 4 | Innovative Microstructural Transformation upon CO2 Supercritical Conditions on Metal-Nucleobase Aerogel and Its Use as Effective Filler for HPLC Biomolecules Separation. Nanomaterials, 2022, 12, 675. | 4.1 | 0 |
| 5 | Engineering Periodic Dinuclear Lanthanideâ€Directed Networks Featuring Tunable Energy Level Alignment and Magnetic Anisotropy by Metal Exchange. Small, 2022, 18, e2107073. | 10.0 | 8 |
| 6 | Metallated Isoindigo–Porphyrin Covalent Organic Framework Photocatalyst with a Narrow Band Gap for Efficient CO ₂ Conversion. ACS Applied Materials & Interfaces, 2022, 14, 2015-2022. | 8.0 | 31 |
| 7 | Concentration asymmetry and carbon enrichment in titanium carbide and silicon carbide clusters. Physical Review A, 2022, 105, . | 2.5 | 2 |
| 8 | From high quality packing to disordered nucleation or phase separation in donor/acceptor interfaces: ClAlPc-C ₆₀ on Au(111). Physical Chemistry Chemical Physics, 2021, 23, 14363-14371. | 2.8 | 1 |
| 9 | Photocatalytic degradation of organic pollutants through conjugated poly(azomethine) networks based on terthiophene–naphthalimide assemblies. RSC Advances, 2021, 11, 2701-2705. | 3.6 | 7 |
| 10 | Copper-assisted oxidation of catechols into quinone derivatives. Chemical Science, 2021, 12, 2257-2267. | 7.4 | 16 |
| 11 | Lanthanide-porphyrin species as Kondo irreversible switches through tip-induced coordination chemistry. Nanoscale, 2021, 13, 8600-8606. | 5.6 | 4 |
| 12 | Dysprosium-directed metallosupramolecular network on graphene/Ir(111). Chemical Communications, 2021, 57, 1380-1383. | 4.1 | 12 |
| 13 | Role of the Structure and Reactivity of Cu and Ag Surfaces in the Formation of a 2D Metal–Hexahydroxytriphenylene Network. Journal of Physical Chemistry C, 2021, 125, 17333-17341. | 3.1 | 12 |
| 14 | Tuning the Magnetic Anisotropy of Lanthanides on a Metal Substrate by Metal–Organic Coordination. Small, 2021, 17, e2102753. | 10.0 | 8 |
| 15 | A Trapezoidal Octacyanoquinoid Acceptor Forms Solution and Surface Products by Antiparallel Shape Fitting with Conformational Dipole Momentum Switch. Angewandte Chemie - International Edition, 2021, 60, 17887-17892. | 13.8 | 5 |
| 16 | Metal-catalyst-free gas-phase synthesis of long-chain hydrocarbons. Nature Communications, 2021, 12, 5937. | 12.8 | 7 |
| 17 | Hydrogen Interaction with Tungsten Disulfide Nanostructures. , 2021, , . | | 0 |
| 18 | Cu(I)–I-2,4-diaminopyrimidine Coordination Polymers with Optoelectronic Properties as a Proof of Concept for Solar Cells. Inorganic Chemistry, 2021, 60, 1208-1219. | 4.0 | 11 |

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| 19 | Oxygen reduction using a metal-free naphthalene diimide-based covalent organic framework electrocatalyst. Chemical Communications, 2020, 56, 1267-1270. | 4.1 | 56 |
| 20 | Cunning defects: emission control by structural point defects on Cu(<scp>i</scp>)I double chain coordination polymers. Journal of Materials Chemistry C, 2020, 8, 1448-1458. | 5.5 | 11 |
| 21 | Oxygen intercalation in PVD graphene grown on copper substrates: A decoupling approach. Applied Surface Science, 2020, 529, 147100. | 6.1 | 10 |
| 22 | Onâ€Surface Driven Formal Michael Addition Produces m â€Polyaniline Oligomers on Pt(111). Angewandte Chemie - International Edition, 2020, 59, 23220-23227. | 13.8 | 5 |
| 23 | On‣urface Driven Formal Michael Addition Produces m â€Polyaniline Oligomers on Pt(111). Angewandte Chemie, 2020, 132, 23420-23427. | 2.0 | 1 |
| 24 | Role of the Metal Surface on the Room Temperature Activation of the Alcohol and Amino Groups of <i>p</i> -Aminophenol. Journal of Physical Chemistry C, 2020, 124, 19655-19665. | 3.1 | 2 |
| 25 | Cathodoluminescence in single and multiwall WS2 nanotubes: Evidence for quantum confinement and strain effect. Applied Physics Reviews, 2020, 7, . | 11.3 | 15 |
| 26 | <i>In silico</i> design of 2D polymers containing truxene-based platforms: insights into their structural and electronic properties. Journal of Materials Chemistry C, 2020, 8, 15416-15425. | 5.5 | 13 |
| 27 | Chemical equilibrium in AGB atmospheres: successes, failures, and prospects for small molecules, clusters, and condensates. Astronomy and Astrophysics, 2020, 637, A59. | 5.1 | 55 |
| 28 | Experimental and Theoretical Study of Dynamic Structural Transformations between Sensing Copper(II)-Uracil Antiferromagnetic and Metamagnetic Coordination Compounds. Crystal Growth and Design, 2020, 20, 5097-5107. | 3.0 | 0 |
| 29 | Production and processing of graphene and related materials. 2D Materials, 2020, 7, 022001. | 4.4 | 333 |
| 30 | Ultra-thin NaCl films as protective layers for graphene. Nanoscale, 2019, 11, 16767-16772. | 5.6 | 6 |
| 31 | Hydrogen quenches the size effects in carbon clusters. Physical Chemistry Chemical Physics, 2019, 21, 10402-10410. | 2.8 | 3 |
| 32 | Reversible transformation between Cu(<scp>i</scp>)-thiophenolate coordination polymers displaying luminescence and electrical properties. CrystEngComm, 2019, 21, 3232-3239. | 2.6 | 10 |
| 33 | Multifunctional Copper(I) Coordination Polymers with Aromatic Mono- and Ditopic Thioamides. Inorganic Chemistry, 2019, 58, 3290-3301. | 4.0 | 42 |
| 34 | Versatile Graphene-Based Platform for Robust Nanobiohybrid Interfaces. ACS Omega, 2019, 4, 3287-3297. | 3.5 | 9 |
| 35 | 3D Printing of a Thermo―and Solvatochromic Composite Material Based on a Cu(II)–Thymine Coordination Polymer with Moisture Sensing Capabilities. Advanced Functional Materials, 2019, 29, 1808424. | 14.9 | 35 |
| 36 | Fluorescence enhancement of fungicide thiabendazole by van der Waals interaction with transition metal dichalcogenide nanosheets for highly specific sensors. Nanoscale, 2019, 11, 23156-23164. | 5.6 | 6 |

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| 37 | On-Surface Hydrogen-Induced Covalent Coupling of Polycyclic Aromatic Hydrocarbons via a Superhydrogenated Intermediate. Journal of the American Chemical Society, 2019, 141, 3550-3557. | 13.7 | 40 |
| 38 | Modelling of adsorption and intercalation of hydrogen on/into tungsten disulphide multilayers and multiwall nanotubes. Physical Chemistry Chemical Physics, 2018, 20, 12061-12074. | 2.8 | 6 |
| 39 | Chemistry below graphene: Decoupling epitaxial graphene from metals by potential-controlled electrochemical oxidation. Carbon, 2018, 129, 837-846. | 10.3 | 30 |
| 40 | Adsorption Geometry and Energy Level Alignment at the PTCDA/TiO2(110) Interface. Journal of Physical Chemistry B, 2018, 122, 534-542. | 2.6 | 11 |
| 41 | Reversible Thermochromic Polymeric Thin Films Made of Ultrathin 2D Crystals of Coordination Polymers Based on Copper(I)â€Thiophenolates. Advanced Functional Materials, 2018, 28, 1704040. | 14.9 | 53 |
| 42 | An improved descriptor of cluster stability: application to small carbon clusters. Physical Chemistry Chemical Physics, 2018, 20, 27368-27374. | 2.8 | 8 |
| 43 | Layer-Stacking-Driven Fluorescence in a Two-Dimensional Imine-Linked Covalent Organic Framework. Journal of the American Chemical Society, 2018, 140, 12922-12929. | 13.7 | 147 |
| 44 | How Au Outperforms Pt in the Catalytic Reduction of Methane Towards Ethane and Molecular Hydrogen. Topics in Catalysis, 2018, 61, 1290-1299. | 2.8 | 0 |
| 45 | Size-Selective Carbon Clusters as Obstacles to Graphene Growth on a Metal. Nano Letters, 2018, 18, 4812-4820. | 9.1 | 7 |
| 46 | Chiral Organization and Charge Redistribution in Chloroaluminum Phthalocyanine on Au(111) Beyond the Monolayer. Journal of Physical Chemistry C, 2018, 122, 16033-16041. | 3.1 | 9 |
| 47 | Onâ€6urface Bottomâ€Up Synthesis of Azine Derivatives Displaying Strong Acceptor Behavior. Angewandte Chemie, 2018, 130, 8718-8722. | 2.0 | 7 |
| 48 | Onâ€Surface Bottomâ€Up Synthesis of Azine Derivatives Displaying Strong Acceptor Behavior. Angewandte Chemie - International Edition, 2018, 57, 8582-8586. | 13.8 | 13 |
| 49 | Smart composite films of nanometric thickness based on copper–iodine coordination polymers. Toward sensors. Chemical Science, 2018, 9, 8000-8010. | 7.4 | 44 |
| 50 | Supramolecular Interactions Modulating Electrical Conductivity and Nanoprocessing of Copper–Iodine Double-Chain Coordination Polymers. Inorganic Chemistry, 2018, 57, 7568-7577. | 4.0 | 22 |
| 51 | Highly selective covalent organic functionalization of epitaxial graphene. Nature Communications, 2017, 8, 15306. | 12.8 | 45 |
| 52 | High-quality PVD graphene growth by fullerene decomposition on Cu foils. Carbon, 2017, 119, 535-543. | 10.3 | 29 |
| 53 | Hydrogen Chemical Configuration and Thermal Stability in Tungsten Disulfide Nanoparticles Exposed to Hydrogen Plasma. Journal of Physical Chemistry C, 2017, 121, 11747-11756. | 3.1 | 6 |
| 54 | Group 10 Metal Benzene-1,2-dithiolate Derivatives in the Synthesis of Coordination Polymers Containing Potassium Countercations. Inorganic Chemistry, 2017, 56, 11810-11818. | 4.0 | 12 |

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| 55 | Multistimuli Response Micro―and Nanolayers of a Coordination Polymer Based on Cu ₂ I ₂ Chains Linked by 2â€Aminopyrazine. Small, 2017, 13, 1700965. | 10.0 | 43 |
| 56 | Spectroscopic characterization of the on-surface induced (cyclo)dehydrogenation of a N-heteroaromatic compound on noble metal surfaces. Physical Chemistry Chemical Physics, 2017, 19, 22454-22461. | 2.8 | 3 |
| 57 | Unveiling universal trends for the energy level alignment in organic/oxide interfaces. Physical Chemistry Chemical Physics, 2017, 19, 24412-24420. | 2.8 | 9 |
| 58 | Low temperature metal free growth of graphene on insulating substrates by plasma assisted chemical vapor deposition. 2D Materials, 2017, 4, 015009. | 4.4 | 38 |
| 59 | Role of the Pinning Points in epitaxial Graphene Moiré Superstructures on the Pt(111) Surface. Scientific Reports, 2016, 6, 20354. | 3.3 | 18 |
| 60 | Luminescent Thermochromism of 2D Coordination Polymers Based on Copper(I) Halides with 4â€Hydroxythiophenol. Chemistry - A European Journal, 2016, 22, 18027-18035. | 3.3 | 43 |
| 61 | Metalation of tetraphenylporphyrin with nickel on a TiO2(110)-1 × 2 surface. Nanoscale, 2016, 8, 1123-1132. | 5.6 | 20 |
| 62 | Adsorption and coupling of 4-aminophenol on Pt(111) surfaces. Surface Science, 2016, 646, 5-12. | 1.9 | 8 |
| 63 | Densely Packed ZnTPPs Monolayer on the Rutile TiO ₂ (110)-(1 × 1) Surface: Adsorption Behavior and Energy Level Alignment. Journal of Physical Chemistry C, 2016, 120, 4430-4437. | 3.1 | 26 |
| 64 | On-Surface (Cyclo-)Dehydrogenation Reactions: Role of Surface Diffusion. Advances in Atom and Single Molecule Machines, 2016, , 43-83. | 0.0 | 2 |
| 65 | Electrical Conductivity and Strong Luminescence in Copper Iodide Double Chains with Isonicotinato Derivatives. Chemistry - A European Journal, 2015, 21, 17282-17292. | 3.3 | 31 |
| 66 | On-surface self-organization of a robust metal–organic cluster based on copper(<scp>i</scp>) with chloride and organosulphur ligands. Chemical Communications, 2015, 51, 3243-3246. | 4.1 | 4 |
| 67 | Mechanical and optical properties of ultralarge flakes of a metal–organic framework with molecular thickness. Chemical Science, 2015, 6, 2553-2558. | 7.4 | 141 |
| 68 | Reversible stimulus-responsive Cu(<scp>i</scp>) iodide pyridine coordination polymer. Chemical Communications, 2015, 51, 14306-14309. | 4.1 | 35 |
| 69 | Ultrafast Atomic Diffusion Inducing a Reversible(23×23)R30°↔(3×3)R30°Transition onSn/Si(111)â^¶B. Pl Review Letters, 2015, 114, 196101. | nysical | 7 |
| 70 | Densely Packed Perylene Layers on the Rutile TiO ₂ (110)-(1 × 1) Surface. Journal of Physical Chemistry C, 2015, 119, 7809-7816. | 3.1 | 11 |
| 71 | Halo and Pseudohalo Cu(I)-Pyridinato Double Chains with Tunable Physical Properties. Inorganic Chemistry, 2015, 54, 10738-10747. | 4.0 | 19 |
| 72 | Chemical Interaction, Space-Charge Layer, and Molecule Charging Energy for a TiO ₂ /TCNQ Interface. Journal of Physical Chemistry C, 2015, 119, 22086-22091. | 3.1 | 9 |

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| 73 | Ortho and Para Hydrogen Dimers on G/SiC(0001): Combined STM and DFT Study. Langmuir, 2015, 31, 233-239. | 3.5 | 12 |
| 74 | Nanostructure Oxide, Metal Oxide and Composite Cylindrical Shapes For Energy and Electromagnetic Spectrum Uses: First Principles Structural, Electronic, and Transport Characterization of SiO2 NanoWires, RuO2 NanoTubes, and SiO2/RuO2 NanoCables. , 2014, , . | | 0 |
| 75 | Etching of Graphene in a Hydrogen-rich Atmosphere toward the Formation of Hydrocarbons in Circumstellar Clouds. Journal of Physical Chemistry C, 2014, 118, 26882-26886. | 3.1 | 9 |
| 76 | Antiphase Boundaries Accumulation Forming a New C ₆₀ Decoupled Crystallographic Phase on the Rutile TiO ₂ (110)-(1 × 1) Surface. Journal of Physical Chemistry C, 2014, 118, 27318-27324. | 3.1 | 5 |
| 77 | Electron transport signature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H<mml:mn>2</mml:mn></mml:mi </mml:msub>dissociation on atomic gold wires. Physical Review B. 2014. 90</mml:math | 3.2 | 4 |
| 78 | Statistical analysis of stretched aluminum nanowires. Journal of Nanoparticle Research, 2014, 16, 1. | 1.9 | 2 |
| 79 | Graphene etching on SiC grains as a path to interstellar polycyclic aromatic hydrocarbons formation. Nature Communications, 2014, 5, 3054. | 12.8 | 59 |
| 80 | Reversible recrystallization process of copper and silver thioacetamide–halide coordination polymers and their basic building blocks. CrystEngComm, 2014, 16, 8224-8231. | 2.6 | 28 |
| 81 | Sequential formation of N-doped nanohelicenes, nanographenes and nanodomes by surface-assisted chemical (cyclo)dehydrogenation of heteroaromatics. Chemical Communications, 2014, 50, 1555. | 4.1 | 23 |
| 82 | Metallicity enhancement in core–shell SiO2@RuO2nanowires. RSC Advances, 2014, 4, 34696-34700. | 3.6 | 1 |
| 83 | Imaging Molecular Orbitals of PTCDA on Graphene on Pt(111): Electronic Structure by STM and First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 12782-12788. | 3.1 | 48 |
| 84 | Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers. Angewandte Chemie - International Edition, 2014, 53, 8316-8319. | 13.8 | 366 |
| 85 | Tailored Formation of N-Doped Nanoarchitectures by Diffusion-Controlled on-Surface (Cyclo)Dehydrogenation of Heteroaromatics. ACS Nano, 2013, 7, 3676-3684. | 14.6 | 52 |
| 86 | Tailoring structural and electronic properties of RuO2 nanotubes: a many-body approach and electronic transport. Physical Chemistry Chemical Physics, 2013, 15, 14715. | 2.8 | 23 |
| 87 | Chemistry and temperature-assisted dehydrogenation of C60H30 molecules on TiO2(110) surfaces. Nanoscale, 2013, 5, 11058. | 5.6 | 17 |
| 88 | Energy Level Alignment in Organic–Organic Heterojunctions: The TTF/TCNQ Interface. Journal of Physical Chemistry C, 2013, 117, 3888-3894. | 3.1 | 14 |
| 89 | Number of outer electrons as descriptor for adsorption processes on transition metals and their oxides. Chemical Science, 2013, 4, 1245. | 7.4 | 273 |
| 90 | Oxygen reduction and evolution at single-metal active sites: Comparison between functionalized graphitic materials and protoporphyrins. Surface Science, 2013, 607, 47-53. | 1.9 | 121 |

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| 91 | Effect of van der Waals forces on the stacking of coronenes encapsulated in a single-wall carbon nanotube and many-body excitation spectrum. Carbon, 2013, 54, 113-123. | 10.3 | 25 |
| 92 | Solventâ€Induced Delamination of a Multifunctional Two Dimensional Coordination Polymer. Advanced Materials, 2013, 25, 2141-2146. | 21.0 | 146 |
| 93 | On the organic energy gap problem. Journal of Physics Condensed Matter, 2013, 25, 094007. | 1.8 | 2 |
| 94 | Barrier height formation in organic blends/metal interfaces: Case of tetrathiafulvalene-tetracyanoquinodimethane/Au(111). Journal of Chemical Physics, 2013, 139, 214706. | 3.0 | 14 |
| 95 | Improvement of Scanning Tunneling Microscopy Resolution with H-Sensitized Tips. Physical Review Letters, 2012, 108, 246102. | 7.8 | 34 |
| 96 | First-Principles Structural and Electronic Characterization of Ordered SiO ₂ Nanowires. Journal of Physical Chemistry C, 2012, 116, 18973-18982. | 3.1 | 22 |
| 97 | Physical and Chemical Nature of the Scaling Relations between Adsorption Energies of Atoms on Metal Surfaces. Physical Review Letters, 2012, 108, 116103. | 7.8 | 233 |
| 98 | Scattering of a proton with the Li4 cluster: Non-adiabatic molecular dynamics description based on time-dependent density-functional theory. Chemical Physics, 2012, 399, 130-134. | 1.9 | 40 |
| 99 | Theoretical characterization of the TTF/Au (111) interface: STM imaging, band alignment and charging energy. Organic Electronics, 2012, 13, 399-408. | 2.6 | 16 |
| 100 | Density functional studies of functionalized graphitic materials with late transition metals for oxygen reduction reactions. Physical Chemistry Chemical Physics, 2011, 13, 15639. | 2.8 | 454 |
| 101 | C6H6/Au(111): Interface dipoles, band alignment, charging energy, and van der Waals interaction. Journal of Chemical Physics, 2011, 134, 044701. | 3.0 | 59 |
| 102 | On the behavior of BrÃ,nsted-Evans-Polanyi relations for transition metal oxides. Journal of Chemical Physics, 2011, 134, 244509. | 3.0 | 128 |
| 103 | Theoretical Study of the Structural Stability and the Electronic Properties of Al _m H _n Clusters. Journal of Computational and Theoretical Nanoscience, 2011, 8, 609-615. | 0.4 | 0 |
| 104 | Barrier height formation for the PTCDA/Au(111) interface. Chemical Physics, 2011, 390, 14-19. | 1.9 | 13 |
| 105 | Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. Journal of Physical Chemistry C, 2011, 115, 2244-2252. | 3.1 | 52 |
| 106 | Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. ChemCatChem, 2011, 3, 1159-1165. | 3.7 | 3,208 |
| 107 | Simulating the organicâ€molecule/metal interface TCNQ/Au(111). Physica Status Solidi (B): Basic Research, 2011, 248, 2044-2049. | 1.5 | 11 |
| 108 | Back Cover: Simulating the organicâ€molecule/metal interface TCNQ/Au(111) (Phys. Status Solidi B 9/2011). Physica Status Solidi (B): Basic Research, 2011, 248, . | 1.5 | 20 |

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| 109 | Trends in Stability of Perovskite Oxides. Angewandte Chemie - International Edition, 2010, 49, 7699-7701. | 13.8 | 98 |
| 110 | Barrier formation and charging energy for a variable nanogap organic molecular junction: a tip/C60/Au(111) configuration. Journal of Physics Condensed Matter, 2010, 22, 304007. | 1.8 | 14 |
| 111 | Optical to ultraviolet spectra of sandwiches of benzene and transition metal atoms: Time dependent density functional theory and many-body calculations. Journal of Chemical Physics, 2010, 132, 044314. | 3.0 | 40 |
| 112 | Formation energies of rutile metal dioxides using density functional theory. Physical Review B, 2009, 79, . | 3.2 | 87 |
| 113 | Optical absorption spectra of Ag11 isomers. European Physical Journal D, 2009, 52, 199-202. | 1.3 | 6 |
| 114 | Adsorption of Lithium on Finite Graphitic Clusters. Journal of Physical Chemistry C, 2009, 113, 939-941. | 3.1 | 34 |
| 115 | Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101. | 3.0 | 77 |
| 116 | Stability and Electronic Properties of TiO ₂ Nanostructures With and Without B and N Doping. Journal of Physical Chemistry C, 2009, 113, 12301-12308. | 3.1 | 102 |
| 117 | Scaling Relationships for Adsorption Energies on Transition Metal Oxide, Sulfide, and Nitride Surfaces. Angewandte Chemie - International Edition, 2008, 47, 4683-4686. | 13.8 | 301 |
| 118 | Electronic and atomic structure of the AlnHn+2 clusters. Journal of Chemical Physics, 2008, 129, 074306. | 3.0 | 15 |
| 119 | Theoretical study of the photoabsorption spectrum of small chromium clusters. Physical Review B, 2007, 76, . | 3.2 | 12 |
| 120 | Theoretical study of molecular hydrogen clusters. European Physical Journal D, 2007, 43, 61-64. | 1.3 | 25 |
| 121 | Optical Absorption Spectra of V ⁺ ₄ Isomers: One Example of First-Principles Theoretical Spectroscopy with Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2006, 3, 761-766. | 0.4 | 8 |
| 122 | Photoabsorption spectra of Ti8C12 metallocarbohedrynes: Theoretical spectroscopy within time-dependent density functional theory. Journal of Chemical Physics, 2006, 125, 074311. | 3.0 | 16 |
| 123 | Optical Absorption Spectra of V ⁺ ₄ Isomers: One Example of First-Principles Theoretical Spectroscopy with Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2006, 3, 761-766. | 0.4 | 8 |
| 124 | Theoretical study of the reactivity of cesium with benzene and graphitic CxHy clusters. Journal of Chemical Physics, 2005, 123, 074303. | 3.0 | 7 |
| 125 | Calculation of the optical spectrum of the Ti8C12 and V8C12 Met-Cars. Chemical Physics Letters, 2004, 398, 292-296. | 2.6 | 12 |
| 126 | Structure, stability and optical absorption spectra of small TinCx clusters: a first-principles approach. Monthly Notices of the Royal Astronomical Society, 0, , . | 4.4 | 6 |