# Gianfranco Pacchioni

List of Publications by Year
in descending order

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|---|---|---|---|
| 596 papers | 36,706 citations | 2797 94 h-index | 5820 161 g-index |
| 638 all docs | 638 docs citations | 638 times ranked | 22807 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | DFT study of electronic properties of N-doped ZnO and ZnO/Cu(111) bilayer films. Surface Science, 2022, 716, 121978. | 0.8 | 10 |
| 2 | From Li clusters to nanocatalysis: A brief tour of 40Âyears of cluster chemistry. Inorganica Chimica Acta, 2022, 530, 120680. | 1.2 | 1 |
| 3 | A DFT study of formic acid decomposition on the stoichiometric SnO2 surface as a function of iso-valent doping. Surface Science, 2022, 718, 122009. | 0.8 | 4 |
| 4 | Density Functional Theory Estimate of Halide Perovskite Band Gap: When Spin Orbit Coupling Helps. Journal of Physical Chemistry C, 2022, 126, 2184-2198. | 1.5 | 40 |
| 5 | LaFeO<sub>3</sub> meets nitrogen-doped graphene functionalized with ultralow Pt loading in an impactful Z-scheme platform for photocatalytic hydrogen evolution. Journal of Materials Chemistry A, 2022, 10, 3330-3340. | 5.2 | 14 |
| 6 | Azide-Alkyne Click Chemistry over a Heterogeneous Copper-Based Single-Atom Catalyst. ACS Catalysis, 2022, 12, 2947-2958. | 5.5 | 68 |
| 7 | First principles approach to solar energy conversion efficiency of semiconductor heterojunctions. Solar Energy, 2022, 236, 445-454. | 2.9 | 6 |
| 8 | Growth of Nâ€Heterocyclic Carbene Assemblies on Cu(100) and Cu(111): From Single Molecules to Magicâ€Number Islands. Angewandte Chemie - International Edition, 2022, 61, . | 7.2 | 13 |
| 9 | Interfacing single-atom catalysis with continuous-flow organic electrosynthesis. Chemical Society Reviews, 2022, 51, 3898-3925. | 18.7 | 50 |
| 10 | Universal Principles for the Rational Design of Single Atom Electrocatalysts? Handle with Care. ACS Catalysis, 2022, 12, 5846-5856. | 5.5 | 60 |
| 11 | Defect engineering of oxide surfaces: dream or reality?. Journal of Physics Condensed Matter, 2022, 34, 291501. | 0.7 | 2 |
| 12 | Magnetic nature and hyperfine interactions of transition metal atoms adsorbed on ultrathin insulating films: a challenge for DFT. Physical Chemistry Chemical Physics, 2022, 24, 15891-15903. | 1.3 | 5 |
| 13 | pH Dependence of MgO, TiO<sub>2</sub>, and Î³-Al<sub>2</sub>O<sub>3</sub> Surface Chemistry from First Principles. Journal of Physical Chemistry C, 2022, 126, 10216-10223. | 1.5 | 21 |
| 14 | Growth and Atomicâ€Scale Characterization of Ultrathin Silica and Germania Films: The Crucial Role of the Metal Support. Chemistry - A European Journal, 2021, 27, 1870-1885. | 1.7 | 13 |
| 15 | Z-Scheme versus type-II junction in g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> and g-C<sub>3</sub>N<sub>4</sub>/SrTiO<sub>3</sub>/TiO<sub>2</sub> heterostructures. Catalysis Science and Technology, 2021, 11, 3589-3598. | 2.1 | 25 |
| 16 | Role of surface termination and quantum size in Î±-CsPbX<sub>3</sub> (X = Cl, Br, I) 2D nanostructures for solar light harvesting. Physical Chemistry Chemical Physics, 2021, 23, 3031-3040. | 1.3 | 20 |
| 17 | Frontispiece: Growth and Atomicâ€Scale Characterization of Ultrathin Silica and Germania Films: The Crucial Role of the Metal Support. Chemistry - A European Journal, 2021, 27, . | 1.7 | 0 |
| 18 | Plasmonic Au nanoclusters dispersed in nitrogen-doped graphene as a robust photocatalyst for light-to-hydrogen conversion. Journal of Materials Chemistry A, 2021, 9, 22810-22819. | 5.2 | 26 |

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| 19 | Structural and electronic properties of TiO2 from first principles calculations. , 2021, , 67-85. | | 2 |
| 20 | Nature and Role of Surface Junctions in BiOIO<sub>3</sub> Photocatalysts. Advanced Functional Materials, 2021, 31, 2009472. | 7.8 | 20 |
| 21 | Role of support in tuning the properties of single atom catalysts: Cu, Ag, Au, Ni, Pd, and Pt adsorption on SiO2/Ru, SiO2/Pt, and SiO2/Si ultrathin films. Journal of Chemical Physics, 2021, 154, 134706. | 1.2 | 6 |
| 22 | Layered oxides as cathode materials for beyond-Li batteries: A computational study of Ca and Al intercalation in bulk V2O5 and MoO3. Computational Materials Science, 2021, 191, 110324. | 1.4 | 15 |
| 23 | Structure and Band Alignment of InP Photocatalysts Passivated by TiO<sub>2</sub> Thin Films. Journal of Physical Chemistry C, 2021, 125, 11620-11627. | 1.5 | 7 |
| 24 | Structures and properties of Pd nanoparticles intercalated in layered TiO2: A computational study. Catalysis Today, 2021, , . | 2.2 | 1 |
| 25 | Cluster Catalysis with Lattice Oxygen: Tracing Oxygen Transport from a Magnetite (001) Support onto Small Pt Clusters. ACS Catalysis, 2021, 11, 9519-9529. | 5.5 | 14 |
| 26 | Continuous network structure of two-dimensional silica across a supporting metal step edge: An atomic scale study. Physical Review Materials, 2021, 5, . | 0.9 | 6 |
| 27 | Band offset in semiconductor heterojunctions. Journal of Physics Condensed Matter, 2021, 33, 415002. | 0.7 | 19 |
| 28 | WO<sub>3</sub>/BiVO<sub>4</sub> Photoanodes: Facets Matching at the Heterojunction and BiVO<sub>4</sub> Layer Thickness Effects. ACS Applied Energy Materials, 2021, 4, 8421-8431. | 2.5 | 22 |
| 29 | Size and Shape Dependence of the Electronic Structure of Gold Nanoclusters on TiO2. Journal of Physical Chemistry Letters, 2021, 12, 8363-8369. | 2.1 | 6 |
| 30 | Rational Design of Semiconductor Heterojunctions for Photocatalysis. Chemistry - A European Journal, 2021, 27, 13306-13317. | 1.7 | 44 |
| 31 | Frontispiece: Rational Design of Semiconductor Heterojunctions for Photocatalysis. Chemistry - A European Journal, 2021, 27, . | 1.7 | 0 |
| 32 | Iso-valent doping of reducible oxides: a comparison of rutile (110) and anatase (101) TiO<sub>2</sub> surfaces. Journal of Physics Condensed Matter, 2021, 33, 494001. | 0.7 | 5 |
| 33 | Steric and Orbital Effects Induced by Isovalent Dopants on the Surface Chemistry of ZrO2. ACS Catalysis, 2021, 11, 554-567. | 5.5 | 15 |
| 34 | Role of surface termination in forming type-II photocatalyst heterojunctions: the case of TiO<sub>2</sub>/BiVO<sub>4</sub>. Journal of Physics Condensed Matter, 2021, 33, 075001. | 0.7 | 18 |
| 35 | Prediction of 2D ferromagnetism and monovalent europium ions in EuBr/graphene heterojunctions. Physical Chemistry Chemical Physics, 2021, 23, 25500-25506. | 1.3 | 6 |
| 36 | Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts. Journal of the American Chemical Society, 2021, 143, 20431-20441. | 6.6 | 77 |

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| 37 | Structural, electronic and photochemical properties of cerium-doped zirconium titanate. Catalysis Today, 2020, 340, 49-57. | 2.2 | 11 |
| 38 | Unraveling the atomic structure, ripening behavior, and electronic structure of supported Au <sub>20</sub> clusters. Science Advances, 2020, 6, eaay4289. | 4.7 | 27 |
| 39 | Quantum confinement in group IIIâ€"V semiconductor 2D nanostructures. Nanoscale, 2020, 12, 17494-17501. | 2.8 | 46 |
| 40 | Influence of Strain on Acidâ€"Basic Properties of Oxide Surfaces. Journal of Physical Chemistry C, 2020, 124, 19126-19135. | 1.5 | 7 |
| 41 | Characterization of Acid and Basic Sites on Zirconia Surfaces and Nanoparticles by Adsorbed Probe Molecules: A Theoretical Study. Topics in Catalysis, 2020, 63, 1717-1730. | 1.3 | 20 |
| 42 | Structure of a Silica Thin Film on Oxidized Cu(111): Conservation of the Honeycomb Lattice and Role of the Interlayer. Journal of Physical Chemistry C, 2020, 124, 20942-20949. | 1.5 | 9 |
| 43 | Bonding Properties of Isolated Metal Atoms on Two-Dimensional Oxides. Journal of Physical Chemistry C, 2020, 124, 20960-20973. | 1.5 | 9 |
| 44 | Chemical Reactivity of Supported ZnO Clusters: Undercoordinated Zinc and Oxygen Atoms as Active Sites. ChemPhysChem, 2020, 21, 2553-2564. | 1.0 | 5 |
| 45 | Precursor chemistry of h-BN: adsorption, desorption, and decomposition of borazine on Pt(110). Physical Chemistry Chemical Physics, 2020, 22, 11704-11712. | 1.3 | 6 |
| 46 | Nature of SrTiO3/TiO2 (anatase) heterostructure from hybrid density functional theory calculations. Journal of Chemical Physics, 2020, 152, 184704. | 1.2 | 23 |
| 47 | Applied vs fundamental research in heterogeneous photocatalysis: problems and perspectives. An introduction to â€˜physical principles of photocatalysisâ€™. Journal of Physics Condensed Matter, 2020, 32, 360301. | 0.7 | 8 |
| 48 | Interface Oxygen Induced Internal Structures of Ultrathin MgO Islands Grown on Ag(100). Journal of Physical Chemistry C, 2020, 124, 8834-8842. | 1.5 | 5 |
| 49 | Band Gap in Magnetic Insulators from a Charge Transition Level Approach. Journal of Chemical Theory and Computation, 2020, 16, 3786-3798. | 2.3 | 22 |
| 50 | Reductant composition influences the coordination of atomically dispersed Rh on anatase TiO<sub>2</sub>. Catalysis Science and Technology, 2020, 10, 1597-1601. | 2.1 | 34 |
| 51 | On the Real Nature of Rh Singleâ€Atom Catalysts Dispersed on the ZrO<sub>2</sub> Surface. ChemCatChem, 2020, 12, 2595-2604. | 1.8 | 23 |
| 52 | Charge Carriers Cascade in a Ternary TiO<sub>2</sub>/TiO<sub>2</sub>/ZnS Heterojunction: A DFT Study. ChemCatChem, 2020, 12, 2097-2105. | 1.8 | 25 |
| 53 | Oxideâ€Supported Gold Clusters and Nanoparticles in Catalysis: A Computational Chemistry Perspective. ChemCatChem, 2019, 11, 73-89. | 1.8 | 37 |
| 54 | Spontaneous Formation of Gold Cluster Anions on ZnO/Cu(111) Bilayer Films. Journal of Physical Chemistry C, 2019, 123, 7644-7653. | 1.5 | 12 |

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| 55 | DFT Study of 17O NMR Spectroscopy Applied to Zirconia Surfaces and Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 21629-21638. | 1.5 | 8 |
| 56 | Solar-driven chemistry: towards new catalytic solutions for a sustainable world. Rendiconti Lincei, 2019, 30, 443-452. | 1.0 | 25 |
| 57 | Theoretical treatment of semiconductor heterojunctions for photocatalysis: the WO<sub>3</sub>/BiVO<sub>4</sub> interface. Journal of Physics Condensed Matter, 2019, 31, 434001. | 0.7 | 16 |
| 58 | Band Gap of 3D Metal Oxides and Quasi-2D Materials from Hybrid Density Functional Theory: Are Dielectric-Dependent Functionals Superior?. Journal of Chemical Theory and Computation, 2019, 15, 6294-6312. | 2.3 | 45 |
| 59 | Formation of Reversible Adducts by Adsorption of Oxygen on Ceâ€"ZrO<sub>2</sub>: An Unusual Î·<sup>2</sup> Ionic Superoxide. Journal of Physical Chemistry C, 2019, 123, 27088-27096. | 1.5 | 14 |
| 60 | Nitrogen doping in coexposed (001)â€"(101) anatase TiO<sub>2</sub> surfaces: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 21497-21505. | 1.3 | 36 |
| 61 | Electronic structure of CuWO<sub>4</sub>: dielectric-dependent, self-consistent hybrid functional study of a Mottâ€"Hubbard type insulator. Journal of Physics Condensed Matter, 2019, 31, 145503. | 0.7 | 8 |
| 62 | Electronic structure of Al, Ga, In and Cu doped ZnO/Cu(111) bilayer films. Physical Chemistry Chemical Physics, 2019, 21, 369-377. | 1.3 | 28 |
| 63 | Structural evolution of atomically dispersed Pt catalysts dictates reactivity. Nature Materials, 2019, 18, 746-751. | 13.3 | 404 |
| 64 | From Crystalline to Amorphous Germania Bilayer Films at the Atomic Scale: Preparation and Characterization. Angewandte Chemie - International Edition, 2019, 58, 10903-10908. | 7.2 | 10 |
| 65 | From Crystalline to Amorphous Germania Bilayer Films at the Atomic Scale: Preparation and Characterization. Angewandte Chemie, 2019, 131, 11019-11024. | 1.6 | 2 |
| 66 | H<sub>2</sub> Adsorption on Wurtzite ZnO and on ZnO/M(111) (M=Cu, Ag and Au) Bilayer Films. ChemNanoMat, 2019, 5, 932-939. | 1.5 | 8 |
| 67 | The epitaxial growth of ZnO films on Cu(111) surface: Thickness dependence. Applied Surface Science, 2019, 483, 133-139. | 3.1 | 11 |
| 68 | Role of Heterojunction in Charge Carrier Separation in Coexposed Anatase (001)â€"(101) Surfaces. Journal of Physical Chemistry Letters, 2019, 10, 2372-2377. | 2.1 | 46 |
| 69 | Nature of Atomically Dispersed Ru on Anatase TiO<sub>2</sub>: Revisiting Old Data Based on DFT Calculations. Journal of Physical Chemistry C, 2019, 123, 7271-7282. | 1.5 | 16 |
| 70 | Structural and electronic properties of bulk and ultrathin layers of V2O5 and MoO3. Computational Materials Science, 2019, 163, 230-240. | 1.4 | 47 |
| 71 | Growth and characterization of Caâ€"Mo mixed oxide films on Mo(001). Journal of Chemical Physics, 2019, 151, 234708. | 1.2 | 4 |
| 72 | 17O NMR as a measure of basicity of alkaline-earth oxide surfaces: A theoretical study. Journal of Chemical Physics, 2019, 151, 224705. | 1.2 | 8 |

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| 73 | Assessing the film-substrate interaction in germania films on reconstructed Au(111). Physical Review B, 2019, 100, . | 1.1 | 4 |
| 74 | Hydrogen Adsorption on Free-Standing and Agâ€"Pt Supported TiO<sub>2</sub> Thin Films. Journal of Physical Chemistry C, 2019, 123, 7952-7960. | 1.5 | 9 |
| 75 | CO Oxidation Promoted by a Pt4/TiO2 Catalyst: Role of Lattice Oxygen at the Metal/Oxide Interface. Catalysis Letters, 2019, 149, 390-398. | 1.4 | 19 |
| 76 | Role of Nanostructuring on the Properties of Oxide Materials: The Case of Zirconia Nanoparticles. European Journal of Inorganic Chemistry, 2019, 2019, 751-761. | 1.0 | 8 |
| 77 | Role of Metal/Oxide Interfaces in Enhancing the Local Oxide Reducibility. Topics in Catalysis, 2019, 62, 1192-1201. | 1.3 | 14 |
| 78 | Determination of Silica and Germania Film Network Structures on Ru(0001) at the Atomic Scale. Journal of Physical Chemistry C, 2019, 123, 7889-7897. | 1.5 | 14 |
| 79 | Atomic structure of a metal-supported two-dimensional germania film. Physical Review B, 2018, 97, . | 1.1 | 16 |
| 80 | Reduced sintering of mass-selected Au clusters on SiO<sub>2</sub>by alloying with Ti: an aberration-corrected STEM and computational study. Nanoscale, 2018, 10, 2363-2370. | 2.8 | 14 |
| 81 | Controlling the charge state of supported nanoparticles in catalysis: lessons from model systems. Chemical Society Reviews, 2018, 47, 8474-8502. | 18.7 | 155 |
| 82 | Evidence of Charge Transfer to Atomic and Molecular Adsorbates on ZnO/X(111) (X = Cu, Ag, Au) Ultrathin Films. Relevance for Cu/ZnO Catalysts. ACS Catalysis, 2018, 8, 4110-4119. | 5.5 | 36 |
| 83 | Nature of Sinteringâ€Resistant, Singleâ€Atom Ru Species Dispersed on Zirconiaâ€Based Catalysts: A DFT and FTIR Study of CO Adsorption. ChemCatChem, 2018, 10, 2634-2645. | 1.8 | 46 |
| 84 | Ultrathin silica films on Pd(111): Structure and adsorption properties. Surface Science, 2018, 678, 118-123. | 0.8 | 25 |
| 85 | CH3Br adsorption on MgO/Mo ultrathin films: A DFT study. Surface Science, 2018, 672-673, 1-6. | 0.8 | 3 |
| 86 | Support effects and reaction mechanism of acetylene trimerization over silica-supported Cu 4 clusters: A DFT study. Surface Science, 2018, 668, 125-133. | 0.8 | 9 |
| 87 | TiO <sub>2</sub> and ZrO <sub>2</sub> in biomass conversion: why catalyst reduction helps. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170056. | 1.6 | 16 |
| 88 | Accuracy of dielectric-dependent hybrid functionals in the prediction of optoelectronic properties of metal oxide semiconductors: a comprehensive comparison with many-bodyGWand experiments. Journal of Physics Condensed Matter, 2018, 30, 044003. | 0.7 | 59 |
| 89 | Nature of stable single atom Pt catalysts dispersed on anatase TiO2. Journal of Catalysis, 2018, 367, 104-114. | 3.1 | 189 |
| 90 | Theory of Ferromagnetism in Reduced ZrO<sub>2â€"x</sub> Nanoparticles. ACS Omega, 2018, 3, 5301-5307. | 1.6 | 38 |

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| 91 | Bending Rigidity of 2D Silica. Physical Review Letters, 2018, 120, 226101. | 2.9 | 17 |
| 92 | CO Oxidation on a Au/TiO<sub>2</sub> Nanoparticle Catalyst via the Au-Assisted Marsâ€"van Krevelen Mechanism. ACS Catalysis, 2018, 8, 6513-6525. | 5.5 | 103 |
| 93 | Origin of Visible Light Photoactivity of the CeO<sub>2</sub>/ZnO Heterojunction. ACS Applied Energy Materials, 2018, 1, 4247-4260. | 2.5 | 60 |
| 94 | Oxygen Vacancy in Wurtzite ZnO and Metal-Supported ZnO/M(111) Bilayer Films (M = Cu, Ag and Au). Journal of Physical Chemistry C, 2018, 122, 20880-20887. | 1.5 | 18 |
| 95 | The Overproduction of Truth. , 2018, , . | | 10 |
| 96 | ZrO2 Nanoparticles: a density functional theory study of structure, properties and reactivity. Rendiconti Lincei, 2017, 28, 19-27. | 1.0 | 15 |
| 97 | Ferromagnetic Interactions in Highly Stable, Partially Reduced TiO<sub>2</sub>: The S=2 State in Anatase. Angewandte Chemie - International Edition, 2017, 56, 2604-2607. | 7.2 | 18 |
| 98 | Fiftyâ€"Fifty Zrâ€"Ti Solid Solution with a TiO<sub>2</sub>-Type Structure: Electronic Structure and Photochemical Properties of Zirconium Titanate ZrTiO<sub>4</sub>. Journal of Physical Chemistry C, 2017, 121, 5487-5497. | 1.5 | 37 |
| 99 | Ferromagnetic Interactions in Highly Stable, Partially Reduced TiO<sub>2</sub>: The S=2 State in Anatase. Angewandte Chemie, 2017, 129, 2648-2651. | 1.6 | 5 |
| 100 | Reducibility of ZrO<sub>2</sub>/Pt<sub>3</sub>Zr and ZrO<sub>2</sub>/Pt 2D films compared to bulk zirconia: a DFT+U study of oxygen removal and H<sub>2</sub>adsorption. Nanoscale, 2017, 9, 6866-6876. | 2.8 | 19 |
| 101 | Influence of surface hydroxylation on the Ru atom diffusion on the ZrO2(101) surface: A DFT study. Surface Science, 2017, 664, 87-94. | 0.8 | 22 |
| 102 | Anchoring Small Au Clusters on the Dehydroxylated and Hydroxylated SiO2 Î±-Quartz (001) Surface via Ti-Alloying. Journal of Physical Chemistry C, 2017, 121, 14717-14724. | 1.5 | 9 |
| 103 | H<sub>2</sub>O Adsorption on WO<sub>3</sub> and WO<sub>3â€"x</sub> (001) Surfaces. ACS Applied Materials & Interfaces, 2017, 9, 23212-23221. | 4.0 | 79 |
| 104 | CO2 Activation and Hydrogenation: A Comparative DFT Study of Ru10/TiO2 and Cu10/TiO2 Model Catalysts. Catalysis Letters, 2017, 147, 1871-1881. | 1.4 | 25 |
| 105 | Size-dependent dissociation of small cobalt clusters on ultrathin NaCl films. Nano Research, 2017, 10, 1832-1839. | 5.8 | 4 |
| 106 | Ferromagnetism in nitrogen-doped BaO: a self-interaction corrected DFT study. Physical Chemistry Chemical Physics, 2017, 19, 3279-3286. | 1.3 | 7 |
| 107 | CO Oxidation on Au Nanoparticles Supported on ZrO<sub>2</sub>: Role of Metal/Oxide Interface and Oxide Reducibility. ChemCatChem, 2017, 9, 1119-1127. | 1.8 | 54 |
| 108 | Reduction of Hydrogenated ZrO<sub>2</sub> Nanoparticles by Water Desorption. ACS Omega, 2017, 2, 3878-3885. | 1.6 | 14 |

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| 109 | Increasing Oxide Reducibility: The Role of Metal/Oxide Interfaces in the Formation of Oxygen Vacancies. ACS Catalysis, 2017, 7, 6493-6513. | 5.5 | 589 |
| 110 | Structure and dynamics of CaO films: A computational study of an effect of external static electric field. Physical Review B, 2017, 95, . | 1.1 | 2 |
| 111 | Trends in Adhesion Energies of Gold on MgO(100), Rutile TiO<sub>2</sub>(110), and CeO<sub>2</sub>(111) Surfaces: A Comparative DFT Study. Journal of Physical Chemistry C, 2017, 121, 28328-28338. | 1.5 | 29 |
| 112 | The photoactive nitrogen impurity in nitrogen-doped zirconium titanate (N-ZrTiO4): a combined electron paramagnetic resonance and density functional theory study. Journal of Materials Chemistry A, 2017, 5, 13062-13071. | 5.2 | 11 |
| 113 | Adsorption and Dimerization of Late Transition Metal Atoms on the Regular and Defective Quartz (001) Surface. Topics in Catalysis, 2017, 60, 459-470. | 1.3 | 13 |
| 114 | Reprint of â€œTheoretical description of metal/oxide interfacial properties: The case of MgO/Ag(001)â€• Applied Surface Science, 2017, 396, 1850-1854. | 3.1 | 0 |
| 115 | CO Adsorption on Graphite-like ZnO Bilayers Supported on Cu(111), Ag(111), and Au(111) Surfaces. Journal of Physical Chemistry C, 2017, 121, 27453-27461. | 1.5 | 34 |
| 116 | Turning a Nonreducible into a Reducible Oxide via Nanostructuring: Opposite Behavior of Bulk ZrO<sub>2</sub> and ZrO<sub>2</sub> Nanoparticles Toward H<sub>2</sub> Adsorption. Journal of Physical Chemistry C, 2016, 120, 15329-15337. | 1.5 | 33 |
| 117 | Magnetic properties of nitrogen-doped ZrO2: Theoretical evidence of absence of room temperature ferromagnetism. Scientific Reports, 2016, 6, 31435. | 1.6 | 23 |
| 118 | Anisotropic Effects of Oxygen Vacancies on Electrochromic Properties and Conductivity of Î³-Monoclinic WO<sub>3</sub>. Journal of Physical Chemistry C, 2016, 120, 11716-11726. | 1.5 | 70 |
| 119 | Role of Structural Flexibility on the Physical and Chemical Properties of Metal-Supported Oxide Ultrathin Films. Springer Series in Materials Science, 2016, , 91-118. | 0.4 | 3 |
| 120 | Size-Dependent Penetration of Gold Nanoclusters through a Defect-Free, Nonporous NaCl Membrane. Nano Letters, 2016, 16, 3063-3070. | 4.5 | 12 |
| 121 | Mechanism of the Cycloâ€Oligomerisation of C<sub>2</sub>H<sub>2</sub> on Anatase TiO<sub>2</sub> (101) and (001) Surfaces and Their Reduction: An Electron Paramagnetic Resonance and Density Functional Theory Study. ChemPlusChem, 2016, 81, 64-72. | 1.3 | 6 |
| 122 | Theoretical description of metal/oxide interfacial properties: The case of MgO/Ag(001). Applied Surface Science, 2016, 390, 578-582. | 3.1 | 21 |
| 123 | Role of Oxide Reducibility in the Deoxygenation of Phenol on Ruthenium Clusters Supported on the Anatase Titania (1â€‰0â€‰1) Surface. ChemCatChem, 2016, 8, 2492-2499. | 1.8 | 43 |
| 124 | Modelling of an ultra-thin silicatene/silicon-carbide hybrid film. Journal of Physics Condensed Matter, 2016, 28, 364005. | 0.7 | 3 |
| 125 | Effect of Nanostructuring on the Reactivity of Zirconia: A DFT+U Study of Au Atom Adsorption. Journal of Physical Chemistry C, 2016, 120, 17604-17612. | 1.5 | 13 |
| 126 | Acetic acid ketonization on tetragonal zirconia: Role of surface reduction. Journal of Catalysis, 2016, 344, 465-473. | 3.1 | 47 |

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| 127 | Dopant-Induced Diffusion Processes at Metalâ€"Oxide Interfaces Studied for Iron- and Chromium-Doped MgO/Mo(001) Model Systems. Journal of Physical Chemistry C, 2016, 120, 13604-13609. | 1.5 | 14 |
| 128 | A DFT study of the acidâ€"base properties of anatase TiO2 and tetragonal ZrO2 by adsorption of CO and CO2 probe molecules. Surface Science, 2016, 652, 163-171. | 0.8 | 74 |
| 129 | Structure and Properties of Zirconia Nanoparticles from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2016, 120, 4392-4402. | 1.5 | 85 |
| 130 | CO adsorption on a silica bilayer supported on Ru(0001). Surface Science, 2016, 648, 2-9. | 0.8 | 29 |
| 131 | A DFT study of Ni clusters deposition on titania and zirconia (101) surfaces. Surface Science, 2016, 646, 230-238. | 0.8 | 22 |
| 132 | Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. Journal of Chemical Physics, 2015, 143, 134702. | 1.2 | 84 |
| 133 | Communication: Hole localization in Al-doped quartz SiO2 within ab initio hybrid-functional DFT. Journal of Chemical Physics, 2015, 143, 111103. | 1.2 | 32 |
| 134 | A DFT Study of the Reactivity of Anatase TiO<sub>2</sub> and Tetragonal ZrO<sub>2</sub> Stepped Surfaces Compared to the Regular (101) Terraces. ChemPhysChem, 2015, 16, 3642-3651. | 1.0 | 21 |
| 135 | Methanol Oxidation Reaction on Î±â€Tungsten Carbide Versus Platinum (1â€‰1â€‰1) Surfaces: A DFT Electrochemical Study. ChemCatChem, 2015, 7, 3533-3543. | 1.8 | 16 |
| 136 | Atomic Scale Structure and Reduction of Cerium Oxide at the Interface with Platinum. Advanced Materials Interfaces, 2015, 2, 1500375. | 1.9 | 25 |
| 137 | Enhanced CO Oxidation on the Oxide/Metal Interface: From Ultraâ€High Vacuum to Nearâ€Atmospheric Pressures. ChemCatChem, 2015, 7, 2620-2627. | 1.8 | 47 |
| 138 | Lateral Manipulation of Atomic Vacancies in Ultrathin Insulating Films. ACS Nano, 2015, 9, 5318-5325. | 7.3 | 17 |
| 139 | Surfaces are different: A perspective on structural, energetic and electronic properties of (001) surfaces of alkaline earth metal oxides as calculated with hybrid density functional theory by Andrew J. Logsdail, David Mora-Fonz, David O. Scanlon, C. Richard A. Catlow, Alexey A. Sokol. Surface Science, 2015, 642, 66-67. | 0.8 | 1 |
| 140 | Nature of Paramagnetic Species in Nitrogen-Doped SnO<sub>2</sub>: A Combined Electron Paramagnetic Resonance and Density Functional Theory Study. Journal of Physical Chemistry C, 2015, 119, 26895-26903. | 1.5 | 18 |
| 141 | Adsorption of Benzene on Cu(100) and on Cu(100) Covered with an Ultrathin NaCl Film: Moleculeâ€"Substrate Interaction and Decoupling. Journal of Physical Chemistry C, 2015, 119, 4062-4071. | 1.5 | 20 |
| 142 | Tuning the charge state of Ag and Au atoms and clusters deposited on oxide surfaces by doping: a DFT study of the adsorption properties of nitrogen- and niobium-doped TiO<sub>2</sub> and ZrO<sub>2</sub>. Physical Chemistry Chemical Physics, 2015, 17, 22342-22360. | 1.3 | 42 |
| 143 | Hydrogen Adsorption, Dissociation, and Spillover on Ru<sub>10</sub> Clusters Supported on Anatase TiO<sub>2</sub> and Tetragonal ZrO<sub>2</sub> (101) Surfaces. ACS Catalysis, 2015, 5, 5486-5495. | 5.5 | 122 |
| 144 | Phonon-Mediated Electron Transport through CaO Thin Films. Physical Review Letters, 2015, 114, 016804. | 2.9 | 12 |

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