# Francesc Illas Riera

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 653 papers | 26,317 citations | 77 h-index | 124 g-index |
| 695 ext. papers | 28,527 ext. citations | 5.2 avg, IF | 7.34 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 653 | Artificial-intelligence-driven discovery of catalyst genes with application to CO activation on semiconductor oxides.. *Nature Communications*, **2022**, 13, 419 | 17.4 | 13 |
| 652 | Catalytic Reduction of Carbon Dioxide on the (001), (011), and (111) Surfaces of TiC and ZrC: A Computational Study.. *Journal of Physical Chemistry C*, **2022**, 126, 5138-5150 | 3.8 | 1 |
| 651 | Challenges of modeling nanostructured materials for photocatalytic water splitting.. *Chemical Society Reviews*, **2022**, | 58.5 | 5 |
| 650 | Tuning the Interfacial Energetics in WO/WO and WO/TiO Heterojunctions by Nanostructure Morphological Engineering. *Journal of Physical Chemistry Letters*, **2021**, 12, 11528-11533 | 6.4 | 3 |
| 649 | Identifying the Atomic Layer Stacking of MoC MXene by Probe Molecule Adsorption.. *Journal of Physical Chemistry C*, **2021**, 125, 26808-26813 | 3.8 | 2 |
| 648 | The Ti2CO2 MXene as a nucleobase 2D sensor: A first-principles study. *Applied Surface Science*, **2021**, 544, 148946 | 6.7 | 5 |
| 647 | Concepts, models, and methods in computational heterogeneous catalysis illustrated through CO2 conversion. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1530 | 7.9 | 11 |
| 646 | Understanding the Structural and Electronic Properties of Photoactive Tungsten Oxide Nanoparticles from Density Functional Theory and Approaches. *Journal of Chemical Theory and Computation*, **2021**, 17, 3462-3470 | 6.4 | 4 |
| 645 | Assessing the Activity of Ni Clusters Supported on TiC(001) toward CO2 and H2 Dissociation. *Journal of Physical Chemistry C*, **2021**, 125, 12019-12027 | 3.8 | 3 |
| 644 | Assigning XPS features in B,N-doped graphene: input from quantum chemical calculations. *Physical Chemistry Chemical Physics*, **2021**, 23, 1558-1565 | 3.6 | 5 |
| 643 | Insights on alkylidene formation on Mo2C: A potential overlap between direct deoxygenation and olefin metathesis. *Journal of Catalysis*, **2021**, 393, 381-389 | 7.3 | 1 |
| 642 | Exfoliation Energy as a Descriptor of MXenes Synthesizability and Surface Chemical Activity. *Nanomaterials*, **2021**, 11, | 5.4 | 8 |
| 641 | Relating X-ray photoelectron spectroscopy data to chemical bonding in MXenes. *Nanoscale Advances*, **2021**, 3, 2793-2801 | 5.1 | 4 |
| 640 | Mo single atoms in the Cu(111) surface as improved catalytic active centers for deoxygenation reactions. *Catalysis Science and Technology*, **2021**, 11, 4969-4978 | 5.5 | 1 |
| 639 | Interaction of First Row Transition Metals with M2C (M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and W) MXenes: A Quest for Single-Atom Catalysts. *Journal of Physical Chemistry C*, **2021**, 125, 2477-2484 | 3.8 | 19 |
| 638 | Understanding the nature and location of hydroxyl groups on hydrated titania nanoparticles. *Nanoscale*, **2021**, 13, 6577-6585 | 7.7 | 9 |
| 637 | Size and Stoichiometry Effects on the Reactivity of MoCy Nanoparticles toward Ethylene. *Journal of Physical Chemistry C*, **2021**, 125, 6287-6297 | 3.8 | 1 |

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| 636 | Supported Molybdenum Carbide Nanoparticles as an Excellent Catalyst for CO2 Hydrogenation. *ACS Catalysis*, **2021**, 11, 9679-9687 | 13.1 | 2 |
| 635 | Carbon Capture and Usage by MXenes. *ACS Catalysis*, **2021**, 11, 11248-11255 | 13.1 | 8 |
| 634 | Importance of the gas-phase error correction for O2 when using DFT to model the oxygen reduction and evolution reactions. *Journal of Electroanalytical Chemistry*, **2021**, 896, 115178 | 4.1 | 10 |
| 633 | Adsorption and Activation of CO on Nitride MXenes: Composition, Temperature, and Pressure effects. *ChemPhysChem*, **2021**, 22, 2456-2463 | 3.2 | 3 |
| 632 | Unravelling Morphological and Topological Energy Contributions of Metal Nanoparticles.. *Nanomaterials*, **2021**, 12, | 5.4 | 37 |
| 631 | MXenes: New Horizons in Catalysis. *ACS Catalysis*, **2020**, 10, 13487-13503 | 13.1 | 87 |
| 630 | Critical Hydrogen Coverage Effect on the Hydrogenation of Ethylene Catalyzed by □MoC(001): An Ab Initio Thermodynamic and Kinetic Study. *ACS Catalysis*, **2020**, 10, 6213-6222 | 13.1 | 12 |
| 629 | Nature of SrTiO/TiO (anatase) heterostructure from hybrid density functional theory calculations. *Journal of Chemical Physics*, **2020**, 152, 184704 | 3.9 | 18 |
| 628 | Morphology of TiO2 Nanoparticles as a Fingerprint for the Transient Absorption Spectra: Implications for Photocatalysis. *Journal of Physical Chemistry C*, **2020**, 124, 11819-11824 | 3.8 | 4 |
| 627 | Ultra-high selectivity biogas upgrading through porous MXenes. *Journal of Materials Chemistry A*, **2020**, 8, 12296-12300 | 13 | 14 |
| 626 | A Semiempirical Method to Detect and Correct DFT-Based Gas-Phase Errors and Its Application in Electrocatalysis. *ACS Catalysis*, **2020**, 10, 6900-6907 | 13.1 | 36 |
| 625 | Multiscale Study of the Mechanism of Catalytic CO2 Hydrogenation: Role of the Ni(111) Facets. *ACS Catalysis*, **2020**, 10, 8077-8089 | 13.1 | 14 |
| 624 | Boosting the activity of transition metal carbides towards methane activation by nanostructuring. *Physical Chemistry Chemical Physics*, **2020**, 22, 7110-7118 | 3.6 | 8 |
| 623 | Designing water splitting catalysts using rules of thumb: advantages, dangers and alternatives. *Physical Chemistry Chemical Physics*, **2020**, 22, 6797-6803 | 3.6 | 32 |
| 622 | Orbitals Permit the Interpretation of Core-Level Spectroscopies in Terms of Chemistry. *Catalysis Letters*, **2020**, 150, 2457-2463 | 2.8 | 8 |
| 621 | Predicting the Effect of Dopants on CO2 Adsorption in Transition Metal Carbides: Case Study on TiC (001). *Journal of Physical Chemistry C*, **2020**, 124, 15969-15976 | 3.8 | 5 |
| 620 | On the use of DFT+U to describe the electronic structure of TiO nanoparticles: (TiO) as a case study. *Journal of Chemical Physics*, **2020**, 152, 244107 | 3.9 | 2 |
| 619 | Explaining Cu@Pt Bimetallic Nanoparticles Activity Based on NO Adsorption. *Chemistry - A European Journal*, **2020**, 26, 11478-11491 | 4.8 | 2 |

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| 618 | Towards understanding the role of carbon atoms on transition metal surfaces: Implications for catalysis. *Applied Surface Science*, **2020**, 513, 145765 | 6.7 | 6 |
| 617 | Critical effect of carbon vacancies on the reverse water gas shift reaction over vanadium carbide catalysts. *Applied Catalysis B: Environmental*, **2020**, 267, 118719 | 21.8 | 30 |
| 616 | Neutral Organic Radical Formation by Chemisorption on Metal Surfaces. *Journal of Physical Chemistry Letters*, **2020**, 11, 3897-3904 | 6.4 | 6 |
| 615 | Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes. *ACS Catalysis*, **2020**, 10, 5049-5056 | 13.1 | 31 |
| 614 | MXenes atomic layer stacking phase transitions and their chemical activity consequences. *Physical Review Materials*, **2020**, 4, | 3.2 | 14 |
| 613 | Comprehensive analysis of the influence of dispersion on group-14 rutile-type solids. *Physical Review Materials*, **2020**, 4, | 3.2 | 1 |
| 612 | Supported Molybdenum Carbide Nanoparticles as Hot Hydrogen Reservoirs for Catalytic Applications. *Journal of Physical Chemistry Letters*, **2020**, 11, 8437-8441 | 6.4 | 3 |
| 611 | Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments. *Applied Catalysis B: Environmental*, **2020**, 264, 118476 | 21.8 | 19 |
| 610 | Investigating the character of excited states in TiO nanoparticles from topological descriptors: implications for photocatalysis. *Physical Chemistry Chemical Physics*, **2020**, 22, 3017-3029 | 3.6 | 12 |
| 609 | First-Principles Calculations on the Adsorption Behavior of Amino Acids on a Titanium Carbide MXene.. *ACS Applied Bio Materials*, **2020**, 3, 5913-5921 | 4.1 | 17 |
| 608 | Bulk (in)stability as a possible source of surface reconstruction. *Physical Chemistry Chemical Physics*, **2020**, 22, 19249-19253 | 3.6 | 4 |
| 607 | Structural, electronic, and magnetic properties of Ni nanoparticles supported on the TiC(001) surface. *Physical Chemistry Chemical Physics*, **2020**, 22, 26145-26154 | 3.6 | 2 |
| 606 | Limitations of the equivalent core model for understanding core-level spectroscopies. *Physical Chemistry Chemical Physics*, **2020**, 22, 22617-22626 | 3.6 | 3 |
| 605 | Generalized gradient approximation adjusted to transition metals properties: Key roles of exchange and local spin density. *Journal of Computational Chemistry*, **2020**, 41, 2598-2603 | 3.5 | 7 |
| 604 | Elucidating the Structure of Ethanol-Producing Active Sites at Oxide-Derived Cu Electrocatalysts. *ACS Catalysis*, **2020**, 10, 10488-10494 | 13.1 | 17 |
| 603 | The nano gold rush: Graphynes as atomic sieves for coinage and Pt-group transition metals. *Applied Surface Science*, **2020**, 499, 143927 | 6.7 | 3 |
| 602 | MXenes as promising catalysts for water dissociation. *Applied Catalysis B: Environmental*, **2020**, 260, 118118 | 21.8 | 49 |
| 601 | Mechanisms of carbon dioxide reduction on strontium titanate perovskites. *Journal of Materials Chemistry A*, **2020**, 8, 9392-9398 | 13 | 12 |

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| 600 | Kinetic Monte Carlo Simulations Unveil Synergic Effects at Work on Bifunctional Catalysts. *ACS Catalysis*, **2019**, 9, 9117-9126 | 13.1 | 16 |
| 599 | Optical Properties and Chemical Ordering of AgPt Nanoalloys: A Computational Study. *Journal of Physical Chemistry C*, **2019**, 123, 25482-25491 | 3.8 | 6 |
| 598 | Surface Activity of Early Transition-Metal Oxycarbides: CO2 Adsorption Case Study. *Journal of Physical Chemistry C*, **2019**, 123, 3664-3671 | 3.8 | 6 |
| 597 | Efficient preparation of TiO nanoparticle models using interatomic potentials. *Journal of Chemical Physics*, **2019**, 150, 214305 | 3.9 | 4 |
| 596 | Differential many-body effects for initial and core ionic states: impact on XPS spectra. *Theoretical Chemistry Accounts*, **2019**, 138, 1 | 1.9 | 5 |
| 595 | CeO(111) electronic reducibility tuned by ultra-small supported bimetallic Pt-Cu clusters. *Physical Chemistry Chemical Physics*, **2019**, 21, 15286-15296 | 3.6 | 13 |
| 594 | Approaching the Quantitative Description of Enantioselective Adsorption by the Density Functional Theory Means. *Journal of Physical Chemistry C*, **2019**, 123, 11714-11722 | 3.8 | 4 |
| 593 | Room Temperature Methane Capture and Activation by Ni Clusters Supported on TiC(001): Effects of Metal-Carbide Interactions on the Cleavage of the C-H Bond. *Journal of the American Chemical Society*, **2019**, 141, 5303-5313 | 16.4 | 33 |
| 592 | Double-well potential energy surface in the interaction between h-BN and Ni(111). *Physical Chemistry Chemical Physics*, **2019**, 21, 10888-10894 | 3.6 | 3 |
| 591 | Effect of electron correlation in the decomposition of core level binding energy shifts into initial and final state contributions. *Physical Chemistry Chemical Physics*, **2019**, 21, 9399-9406 | 3.6 | 2 |
| 590 | Correcting Flaws in the Assignment of Nitrogen Chemical Environments in N-Doped Graphene. *Journal of Physical Chemistry C*, **2019**, 123, 11319-11327 | 3.8 | 21 |
| 589 | Understanding the interplay between size, morphology and energy gap in photoactive TiO nanoparticles. *Nanoscale*, **2019**, 11, 9032-9041 | 7.7 | 29 |
| 588 | Affordable Estimation of Solvation Contributions to the Adsorption Energies of Oxygenates on Metal Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 5578-5582 | 3.8 | 31 |
| 587 | Electronic Properties of Realistic Anatase TiO Nanoparticles from Calculations on a Gaussian and Plane Waves Scheme. *Journal of Chemical Theory and Computation*, **2019**, 15, 5024-5030 | 6.4 | 5 |
| 586 | Approaching multiplet splitting in X-ray photoelectron spectra by density functional theory methods: NO and O2 molecules as examples. *Chemical Physics Letters*, **2019**, 731, 136617 | 2.5 | 2 |
| 585 | Implicit solvent effects in the determination of Brønsted-Evans-Polanyi relationships for heterogeneously catalyzed reactions. *Physical Chemistry Chemical Physics*, **2019**, 21, 17687-17695 | 3.6 | 3 |
| 584 | Grazynes: Carbon-Based Two-Dimensional Composites with Anisotropic Properties. *Journal of Physical Chemistry C*, **2019**, 123, 27140-27149 | 3.8 | 8 |
| 583 | Assessing the usefulness of transition metal carbides for hydrogenation reactions. *Chemical Communications*, **2019**, 55, 12797-12800 | 5.8 | 16 |

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| 582 | Thickness biased capture of CO on carbide MXenes. *Physical Chemistry Chemical Physics*, **2019**, 21, 23136-23142 | 3.6 | 31 |
| 581 | Subsurface Carbon: A General Feature of Noble Metals. *Angewandte Chemie - International Edition*, **2019**, 58, 1744-1748 | 16.4 | 20 |
| 580 | Subsurface Carbon: A General Feature of Noble Metals. *Angewandte Chemie*, **2019**, 131, 1758-1762 | 3.6 | 5 |
| 579 | Combining Theory and Experiment for Multitechnique Characterization of Activated CO2 on Transition Metal Carbide (001) Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 7567-7576 | 3.8 | 14 |
| 578 | Post-B3LYP Functionals Do Not Improve the Description of Magnetic Coupling in Cu(II) Dinuclear Complexes. *Journal of Physical Chemistry A*, **2018**, 122, 3423-3432 | 2.8 | 7 |
| 577 | CO2 abatement using two-dimensional MXene carbides. *Journal of Materials Chemistry A*, **2018**, 6, 3381-3385 | 9.9 | 93 |
| 576 | Biogas Upgrading by Transition Metal Carbides. *ACS Applied Energy Materials*, **2018**, 1, 43-47 | 6.1 | 15 |
| 575 | Assessing GW Approaches for Predicting Core Level Binding Energies. *Journal of Chemical Theory and Computation*, **2018**, 14, 877-883 | 6.4 | 37 |
| 574 | Properties of Single Oxygen Vacancies on a Realistic (TiO2)84 Nanoparticle: A Challenge for Density Functionals. *Journal of Physical Chemistry C*, **2018**, 122, 2413-2421 | 3.8 | 18 |
| 573 | On the H interactions with transition metal adatoms supported on graphene: a systematic density functional study. *Physical Chemistry Chemical Physics*, **2018**, 20, 3819-3830 | 3.6 | 14 |
| 572 | Electronic and structural properties of Li @Be B (n = 1-14) and Li @Be B (n = 1-21) nanoflakes shed light on possible anode materials for Li-based batteries. *Journal of Computational Chemistry*, **2018**, 39, 1795-1805 | 3.5 | 3 |
| 571 | On the prediction of core level binding energies in molecules, surfaces and solids. *Physical Chemistry Chemical Physics*, **2018**, 20, 8403-8410 | 3.6 | 35 |
| 570 | Matildite Contact with Media: First-Principles Study of AgBiS Surfaces and Nanoparticle Morphology. *Journal of Physical Chemistry B*, **2018**, 122, 521-526 | 3.4 | 7 |
| 569 | General concepts, assumptions, drawbacks, and misuses in kinetic Monte Carlo and microkinetic modeling simulations applied to computational heterogeneous catalysis. *International Journal of Quantum Chemistry*, **2018**, 118, e25518 | 2.1 | 19 |
| 568 | Understanding W Doping in Wurtzite ZnO. *Journal of Physical Chemistry C*, **2018**, 122, 19082-19089 | 3.8 | 3 |
| 567 | CO interaction with violarite (FeNiS) surfaces: a dispersion-corrected DFT study. *Physical Chemistry Chemical Physics*, **2018**, 20, 20439-20446 | 3.6 | 13 |
| 566 | Theoretical Modeling of Electronic Excitations of Gas-Phase and Solvated TiO Nanoclusters and Nanoparticles of Interest in Photocatalysis. *Journal of Chemical Theory and Computation*, **2018**, 14, 4391-4404 | 6.4 | 16 |
| 565 | Robustness of surface activity electronic structure-based descriptors of transition metals. *Physical Chemistry Chemical Physics*, **2018**, 20, 20548-20554 | 3.6 | 8 |

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| 564 | Tuning transition metal carbide activity by surface metal alloying: a case study on CO capture and activation. *Physical Chemistry Chemical Physics*, **2018**, 20, 22179-22186 | 3.6 | 8 |
| 563 | Jacob's Ladder as Sketched by Escher: Assessing the Performance of Broadly Used Density Functionals on Transition Metal Surface Properties. *Journal of Chemical Theory and Computation*, **2018**, 14, 395-403 | 6.4 | 44 |
| 562 | Diversity of Adsorbed Hydrogen on the TiC(001) Surface at High Coverages. *Journal of Physical Chemistry C*, **2018**, 122, 28013-28020 | 3.8 | 12 |
| 561 | Assessing the Performance of Cobalt Phthalocyanine Nanoflakes as Molecular Catalysts for Li-Promoted Oxalate Formation in Li□CO2□Oxalate Batteries. *Journal of Physical Chemistry C*, **2018**, 122, 25776-25784 | 3.8 | 14 |
| 560 | Simulating heterogeneous catalysis on metallic nanoparticles: From under-coordinated sites to extended facets. *Frontiers of Nanoscience*, **2018**, 101-128 | 0.7 | 1 |
| 559 | Modeling realistic titania nanoparticles. *Frontiers of Nanoscience*, **2018**, 12, 205-238 | 0.7 | 1 |
| 558 | Two-dimensional nitrides as highly efficient potential candidates for CO capture and activation. *Physical Chemistry Chemical Physics*, **2018**, 20, 17117-17124 | 3.6 | 33 |
| 557 | Reliable and computationally affordable prediction of the energy gap of (TiO) (10 □h □563) nanoparticles from density functional theory. *Physical Chemistry Chemical Physics*, **2018**, 20, 18907-18911 | 3.6 | 11 |
| 556 | Carbon dissolution and segregation in platinum. *Catalysis Science and Technology*, **2017**, 7, 807-816 | 5.5 | 10 |
| 555 | Adding Pieces to the CO/Pt(111) Puzzle: The Role of Dispersion. *Journal of Physical Chemistry C*, **2017**, 121, 3970-3977 | 3.8 | 31 |
| 554 | Influence of NO and (NO) adsorption on the properties of Fe-N4 porphyrin-like graphene sheets. *Physical Chemistry Chemical Physics*, **2017**, 19, 3201-3213 | 3.6 | 20 |
| 553 | Electronic structure of stoichiometric and reduced ZnO from periodic relativistic all electron hybrid density functional calculations using numeric atom-centered orbitals. *Journal of Computational Chemistry*, **2017**, 38, 523-529 | 3.5 | 13 |
| 552 | ZrO2 Nanoparticles: a density functional theory study of structure, properties and reactivity. *Rendiconti Lincei*, **2017**, 28, 19-27 | 1.7 | 11 |
| 551 | When Anatase Nanoparticles Become Bulklike: Properties of Realistic TiO Nanoparticles in the 1-6 nm Size Range from All Electron Relativistic Density Functional Theory Based Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 1785-1793 | 6.4 | 70 |
| 550 | Systematic study of the effect of HSE functional internal parameters on the electronic structure and band gap of a representative set of metal oxides. *Journal of Computational Chemistry*, **2017**, 38, 781-789 | 3.5 | 47 |
| 549 | Selectivity for CO2 over CH4 on a functionalized periodic mesoporous phenylene-silica explained by transition state theory. *Chemical Physics Letters*, **2017**, 671, 161-164 | 2.5 | 12 |
| 548 | Functionalization of □graphyne by transition metal adatoms. *Carbon*, **2017**, 120, 63-70 | 10.4 | 55 |
| 547 | Effective and Highly Selective CO Generation from CO2 Using a Polycrystalline □Mo2C Catalyst. *ACS Catalysis*, **2017**, 7, 4323-4335 | 13.1 | 68 |

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|---|---|---|---|
| 546 | Highly active Au/δ-MoC and Au/β-Mo2C catalysts for the low-temperature water gas shift reaction: effects of the carbide metal/carbon ratio on the catalyst performance. *Catalysis Science and Technology*, **2017**, 7, 5332-5342 | 5.5 | 26 |
| 545 | Cohesion and coordination effects on transition metal surface energies. *Surface Science*, **2017**, 664, 45-49 | 2.8 | 15 |
| 544 | ZnO powders as multi-facet single crystals. *Physical Chemistry Chemical Physics*, **2017**, 19, 10622-10628 | 3.6 | 10 |
| 543 | Predicting core level binding energies shifts: Suitability of the projector augmented wave approach as implemented in VASP. *Journal of Computational Chemistry*, **2017**, 38, 518-522 | 3.5 | 34 |
| 542 | Adsorption of CO on the rutile TiO(110) surface: a dispersion-corrected density functional theory study. *Physical Chemistry Chemical Physics*, **2017**, 19, 2487-2494 | 3.6 | 8 |
| 541 | Bandgap engineering by cationic disorder: case study on AgBiS. *Physical Chemistry Chemical Physics*, **2017**, 19, 27940-27944 | 3.6 | 16 |
| 540 | Size-Dependent Level Alignment between Rutile and Anatase TiO Nanoparticles: Implications for Photocatalysis. *Journal of Physical Chemistry Letters*, **2017**, 8, 5593-5598 | 6.4 | 62 |
| 539 | Computational materials: Open data settled in materials theory. *Nature*, **2017**, 548, 523 | 50.4 | 6 |
| 538 | Assessing the ability of DFT methods to describe static electron correlation effects: CO core level binding energies as a representative case. *Journal of Chemical Physics*, **2017**, 147, 024106 | 3.9 | 8 |
| 537 | Reduction of Hydrogenated ZrO Nanoparticles by Water Desorption. *ACS Omega*, **2017**, 2, 3878-3885 | 3.9 | 9 |
| 536 | An Empirical, yet Practical Way To Predict the Band Gap in Solids by Using Density Functional Band Structure Calculations. *Journal of Physical Chemistry C*, **2017**, 121, 18862-18866 | 3.8 | 106 |
| 535 | Calix[n]arene-based polyradicals: enhancing ferromagnetism by avoiding edge effects. *Physical Chemistry Chemical Physics*, **2017**, 19, 24264-24270 | 3.6 | 5 |
| 534 | Existence of multi-radical and closed-shell semiconducting states in post-graphene organic Dirac materials. *Nature Communications*, **2017**, 8, 1957 | 17.4 | 38 |
| 533 | Performance of the GW Method in Predicting the Electronic Gap of TiO Nanoparticles. *Journal of Chemical Theory and Computation*, **2017**, 13, 3746-3753 | 6.4 | 16 |
| 532 | Size dependent structural and polymorphic transitions in ZnO: from nanocluster to bulk. *Nanoscale*, **2017**, 9, 10067-10074 | 7.7 | 42 |
| 531 | Substrate-mediated single-atom isolation: dispersion of Ni and La on γ-graphyne. *Theoretical Chemistry Accounts*, **2017**, 136, 1 | 1.9 | 9 |
| 530 | Predicting size-dependent emergence of crystallinity in nanomaterials: titania nanoclusters versus nanocrystals. *Nanoscale*, **2017**, 9, 1049-1058 | 7.7 | 59 |
| 529 | Adsorption and dissociation of molecular hydrogen on orthorhombic β-Mo2C and cubic δ-MoC (001) surfaces. *Surface Science*, **2017**, 656, 24-32 | 1.8 | 34 |

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| 528 | The contact of graphene with Ni(111) surface: description by modern dispersive forces approaches. *Theoretical Chemistry Accounts*, **2016**, 135, 1 | 1.9 | 14 |
| 527 | 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 | 3.8 | 10 |
| 526 | Highly Active Au/EMoC and Cu/EMoC Catalysts for the Conversion of CO2: The Metal/C Ratio as a Key Factor Defining Activity, Selectivity, and Stability. *Journal of the American Chemical Society*, **2016**, 138, 8269-78 | 16.4 | 92 |
| 525 | Transition metal carbides as novel materials for CO2 capture, storage, and activation. *Energy and Environmental Science*, **2016**, 9, 141-144 | 35.4 | 115 |
| 524 | Kinetic Monte Carlo simulations of the water gas shift reaction on Cu(1 1 1) from density functional theory based calculations. *Journal of Catalysis*, **2016**, 333, 217-226 | 7.3 | 38 |
| 523 | Performance of Minnesota functionals on predicting core-level binding energies of molecules containing main-group elements. *Theoretical Chemistry Accounts*, **2016**, 135, 1 | 1.9 | 16 |
| 522 | Structure and Properties of Zirconia Nanoparticles from Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2016**, 120, 4392-4402 | 3.8 | 66 |
| 521 | The conversion of CO2 to methanol on orthorhombic EMo2C and Cu/EMo2C catalysts: mechanism for admetal induced change in the selectivity and activity. *Catalysis Science and Technology*, **2016**, 6, 6766-6777 | 5.5 | 74 |
| 520 | Performance of the TPSS Functional on Predicting Core Level Binding Energies of Main Group Elements Containing Molecules: A Good Choice for Molecules Adsorbed on Metal Surfaces. *Journal of Chemical Theory and Computation*, **2016**, 12, 324-31 | 6.4 | 32 |
| 519 | Unexpectedly large impact of van der Waals interactions on the description of heterogeneously catalyzed reactions: the water gas shift reaction on Cu(321) as a case example. *Physical Chemistry Chemical Physics*, **2016**, 18, 2792-801 | 3.6 | 20 |
| 518 | On the hydrogen adsorption and dissociation on Cu surfaces and nanorows. *Surface Science*, **2016**, 646, 221-229 | 1.8 | 25 |
| 517 | Role of structural symmetry breaking in the structurally induced robust superlubricity of graphene and h-BN homo- and hetero-junctions. *Carbon*, **2016**, 96, 911-918 | 10.4 | 10 |
| 516 | Effect of Size and Structure on the Ground-State and Excited-State Electronic Structure of TiO2 Nanoparticles. *Journal of Chemical Theory and Computation*, **2016**, 12, 3751-63 | 6.4 | 43 |
| 515 | Consequences of electron correlation for XPS binding energies: Representative case for C(1s) and O(1s) XPS of CO. *Journal of Chemical Physics*, **2016**, 145, 144303 | 3.9 | 17 |
| 514 | Matildite versus schapbachite: First-principles investigation of the origin of photoactivity in AgBiS2. *Physical Review B*, **2016**, 94, | 3.3 | 29 |
| 513 | Helical Folding-Induced Stabilization of Ferromagnetic Polyradicals Based on Triarylmethyl Radical Derivatives. *Journal of the American Chemical Society*, **2016**, 138, 5271-5 | 16.4 | 8 |
| 512 | Performance of a modified hybrid functional in the simultaneous description of stoichiometric and reduced TiO2 polymorphs. *Physical Chemistry Chemical Physics*, **2016**, 18, 12357-67 | 3.6 | 37 |
| 511 | Magnetic Coupling Constants in Three Electrons Three Centers Problems from Effective Hamiltonian Theory and Validation of Broken Symmetry-Based Approaches. *Journal of Chemical Theory and Computation*, **2016**, 12, 3228-35 | 6.4 | 6 |

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| 510 | High efficiency of Pt2+- CeO2 novel thin film catalyst as anode for proton exchange membrane fuel cells. *Applied Catalysis B: Environmental*, **2016**, 197, 262-270 | 21.8 | 37 |
| 509 | Effect of the Exchange-Correlation Potential on the Transferability of Br□sted-Evans-Polanyi Relationships in Heterogeneous Catalysis. *Journal of Chemical Theory and Computation*, **2016**, 12, 2121-6 | 6.4 | 15 |
| 508 | Single oxygen vacancies of (TiO2)35 as a prototype reduced nanoparticle: implication for photocatalytic activity. *Physical Chemistry Chemical Physics*, **2016**, 18, 23755-62 | 3.6 | 28 |
| 507 | Comparing the catalytic activity of the water gas shift reaction on Cu(3 2 1) and Cu(1 1 1) surfaces: Step sites do not always enhance the overall reactivity. *Journal of Catalysis*, **2016**, 342, 75-83 | 7.3 | 25 |
| 506 | Handling Magnetic Coupling in Trinuclear Cu(II) Complexes. *Journal of Chemical Theory and Computation*, **2015**, 11, 3650-60 | 6.4 | 11 |
| 505 | Theoretical study of electronic and tribological properties of h-BNC2/graphene, h-BNC2/h-BN and h-BNC2/h-BNC2 bilayers. *Physical Chemistry Chemical Physics*, **2015**, 17, 12908-18 | 3.6 | 6 |
| 504 | Conditional Born-Oppenheimer Dynamics: Quantum Dynamics Simulations for the Model Porphine. *Journal of Physical Chemistry Letters*, **2015**, 6, 1529-35 | 6.4 | 20 |
| 503 | Morphology effects in photoactive ZnO nanostructures: photooxidative activity of polar surfaces. *Journal of Materials Chemistry A*, **2015**, 3, 8782-8792 | 13 | 31 |
| 502 | Electronic-structure-based material descriptors: (in)dependence on self-interaction and Hartree-Fock exchange. *Chemical Communications*, **2015**, 51, 5602-5 | 5.8 | 17 |
| 501 | Structure and electronic properties of Cu nanoclusters supported on Mo2C(001) and MoC(001) surfaces. *Journal of Chemical Physics*, **2015**, 143, 114704 | 3.9 | 22 |
| 500 | Adsorption properties of trifluoroacetic acid on anatase (101) and (001) surfaces: a density functional theory study. *Physical Chemistry Chemical Physics*, **2015**, 17, 23627-33 | 3.6 | 4 |
| 499 | Prediction of core level binding energies in density functional theory: Rigorous definition of initial and final state contributions and implications on the physical meaning of Kohn-Sham energies. *Journal of Chemical Physics*, **2015**, 142, 214102 | 3.9 | 47 |
| 498 | Transition metal adatoms on graphene: A systematic density functional study. *Carbon*, **2015**, 95, 525-534 | 10.4 | 103 |
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