# Javier FernÃ¡ndez Sanz

List of Publications by Year
in descending order

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|---|---|---|---|
| 206 papers | 8,915 citations | 43973 48 h-index | 49773 87 g-index |
| 216 all docs | 216 docs citations | 216 times ranked | 9761 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Catalytic activity of PtCu intermetallic compound for CO oxidation: A theoretical insight. Catalysis Today, 2022, 383, 339-344. | 2.2 | 2 |
| 2 | Optoelectronic properties of Ag2S/graphene and FeS2/graphene nanostructures and interfaces: A density functional study including dispersion forces. Journal of Materials Research, 2022, 37, 1047-1058. | 1.2 | 2 |
| 3 | Charting the Lattice Thermal Conductivities of Iâ€“IIIâ€“VI<sub>2</sub> Chalcopyrite Semiconductors. Chemistry of Materials, 2022, 34, 2833-2841. | 3.2 | 22 |
| 4 | Connecting experimental synthetic variables with the microstructure and electronic properties of doped ferroelectric perovskites for solar cell applications using high-throughput frameworks. Acta Materialia, 2021, 204, 116466. | 3.8 | 4 |
| 5 | High-Throughput Screening of the Thermoelastic Properties of Ultrahigh-Temperature Ceramics. ACS Applied Materials & Interfaces, 2021, 13, 29843-29857. | 4.0 | 8 |
| 6 | Adsorption and activation of CO2 on Pt/CeOx/TiO2(110): Role of the Pt-CeOx interface. Surface Science, 2021, 710, 121852. | 0.8 | 5 |
| 7 | Nanoimaging of Organic Charge Retention Effects: Implications for Nonvolatile Memory, Neuromorphic Computing, and High Dielectric Breakdown Devices. ACS Applied Nano Materials, 2019, 2, 4711-4716. | 2.4 | 4 |
| 8 | Waterâ€“Gas Shift Reaction on K/Cu(111) and Cu/K/TiO<sub>2</sub>(110) Surfaces: Alkali Promotion of Water Dissociation and Production of H<sub>2</sub>. ACS Catalysis, 2019, 9, 10751-10760. | 5.5 | 38 |
| 9 | Electronic structure and adsorption geometry of Pt and Pd metal complexes with 1,3-dithiole-2-thione-4,5-dithiolate ligand on TiO2(101) surface from first-principles calculations. Theoretical Chemistry Accounts, 2019, 138, 1. | 0.5 | 2 |
| 10 | Comprehensive Experimental and Theoretical Study of the CO + NO Reaction Catalyzed by Au/Ni Nanoparticles. ACS Catalysis, 2019, 9, 4919-4929. | 5.5 | 22 |
| 11 | Understanding the Photocatalytic Properties of Pt/CeO<sub>x</sub>/TiO<sub>2</sub>: Structural Effects on Electronic and Optical Properties. ChemPhysChem, 2019, 20, 1624-1629. | 1.0 | 8 |
| 12 | Photo-sensitizing thin-film ferroelectric oxides using materials databases and high-throughput calculations. Journal of Materials Chemistry A, 2019, 7, 27323-27333. | 5.2 | 12 |
| 13 | TiO2 nanotubes sensitized with CdSe quantum dots. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 2 |
| 14 | Adsorption of Prototypical Asphaltenes on Silica: First-Principles DFT Simulations Including Dispersion Corrections. Journal of Physical Chemistry B, 2018, 122, 618-624. | 1.2 | 21 |
| 15 | Analysis of the variables that modify the robustness of Ti-SiO2 catalysts for alkene epoxidation: Role of silylation, deactivation and potential solutions. Molecular Catalysis, 2018, 459, 55-60. | 1.0 | 9 |
| 16 | Graphene Translucency and Interfacial Interactions in the Gold/Graphene/SiC System. Journal of Physical Chemistry Letters, 2018, 9, 3850-3855. | 2.1 | 19 |
| 17 | Improving the activity of gold nanoparticles for the water-gas shift reaction using TiO<sub>2</sub>â€“Y<sub>2</sub>O<sub>3</sub>: an example of catalyst design. Physical Chemistry Chemical Physics, 2018, 20, 22076-22083. | 1.3 | 8 |
| 18 | Structural and electronic properties of lead sulfide quantum dots from screened hybrid density functional calculations including spinâ€“orbit coupling effects. Theoretical Chemistry Accounts, 2017, 136, 1. | 0.5 | 3 |

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| 19 | Effects of the capping ligands, linkers and oxide surface on the electron injection mechanism of copper sulfide quantum dot-sensitized solar cells. Physical Chemistry Chemical Physics, 2017, 19, 14580-14587. | 1.3 | 12 |
| 20 | Molecular dynamics simulations of the role of salinity and temperature on the hydrocarbon/water interfacial tension. Theoretical Chemistry Accounts, 2017, 136, 1. | 0.5 | 16 |
| 21 | First-principles study of nickel complex with 1,3-dithiole-2-thione-4,5-dithiolate ligands as model photosensitizers. Theoretical Chemistry Accounts, 2017, 136, 1. | 0.5 | 7 |
| 22 | Critical Role of Oxygen in Silver-Catalyzed Glaserâ€“Hay Coupling on Ag(100) under Vacuum and in Solution on Ag Particles. ACS Catalysis, 2017, 7, 3113-3120. | 5.5 | 8 |
| 23 | Ag<sub>2</sub>S Quantum Dot-Sensitized Solar Cells by First Principles: The Effect of Capping Ligands and Linkers. Journal of Physical Chemistry A, 2017, 121, 7290-7296. | 1.1 | 17 |
| 24 | Potassium and Water Coadsorption on TiO<sub>2</sub>(110): OH-Induced Anchoring of Potassium and the Generation of Single-Site Catalysts. Journal of Physical Chemistry Letters, 2016, 7, 3866-3872. | 2.1 | 14 |
| 25 | Inverse Oxide/Metal Catalysts in Fundamental Studies and Practical Applications: A Perspective of Recent Developments. Journal of Physical Chemistry Letters, 2016, 7, 2627-2639. | 2.1 | 120 |
| 26 | Cu Deposited on CeOx-Modified TiO<sub>2</sub>(110): Synergistic Effects at the Metalâ€“Oxide Interface and the Mechanism of the WGS Reaction. ACS Catalysis, 2016, 6, 4608-4615. | 5.5 | 43 |
| 27 | Visible Light-Driven H<sub>2</sub> Production over Highly Dispersed Ruthenia on Rutile TiO<sub>2</sub> Nanorods. ACS Catalysis, 2016, 6, 407-417. | 5.5 | 71 |
| 28 | Structural, electronic and optical properties of copper, silver and gold sulfide: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1. | 0.5 | 35 |
| 29 | Adsorption of prototypical amino acids on silica: Influence of the pre-adsorbed water multilayer. Surface Science, 2016, 646, 239-246. | 0.8 | 10 |
| 30 | Graphenes as Efficient Metalâ€Free Fenton Catalysts. Chemistry - A European Journal, 2015, 21, 11966-11971. | 1.7 | 87 |
| 31 | Sonogashira Cross-Coupling and Homocoupling on a Silver Surface: Chlorobenzene and Phenylacetylene on Ag(100). Journal of the American Chemical Society, 2015, 137, 940-947. | 6.6 | 50 |
| 32 | Effect of Capping Ligands and TiO<sub>2</sub> Supporting on the Optical Properties of a (CdSe)<sub>13</sub> Cluster. Journal of Physical Chemistry A, 2015, 119, 1218-1227. | 1.1 | 16 |
| 33 | When ruthenia met titania: achieving extraordinary catalytic activity at low temperature by nanostructuring of oxides. Physical Chemistry Chemical Physics, 2015, 17, 26813-26818. | 1.3 | 0 |
| 34 | Designing a new generation of catalysts: Water gas shift reaction example. Catalysis Today, 2015, 240, 214-219. | 2.2 | 29 |
| 35 | Unraveling the Nature of the Oxideâ€“Metal Interaction in Ceria-Based Noble Metal Inverse Catalysts. Journal of Physical Chemistry C, 2014, 118, 26931-26938. | 1.5 | 33 |
| 36 | Surface oxygen vacancies in gold based catalysts for CO oxidation. RSC Advances, 2014, 4, 13145-13152. | 1.7 | 24 |

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| 37 | The Flexible Surface Revisited: Adsorbate-Induced Reconstruction, Homocoupling, and Sonogashira Cross-Coupling on the Au(100) Surface. Journal of Physical Chemistry C, 2014, 118, 11677-11684. | 1.5 | 31 |
| 38 | Highly active copper-ceria and copper-ceria-titania catalysts for methanol synthesis from CO <sub>2</sub>. Science, 2014, 345, 546-550. | 6.0 | 1,114 |
| 39 | Understanding the Interplay of Dopants, Interfaces, and Anionic Conductivity in Doped Ceria/Zirconia Heteroepitaxial Structures. Chemistry of Materials, 2014, 26, 3385-3390. | 3.2 | 16 |
| 40 | Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Highlights in Theoretical Chemistry, 2014, , 177-183. | 0.0 | 0 |
| 41 | Simulating the optical properties of CdSe clusters using the RT-TDDFT approach. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 27 |
| 42 | Analysis of the origin of lateral interactions in the adsorption of small organic molecules on oxide surfaces. Theoretical Chemistry Accounts, 2013, 132, 1. | 0.5 | 5 |
| 43 | Nature of the Mixed-Oxide Interface in Ceriaâ€“Titania Catalysts: Clusters, Chains, and Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 14463-14471. | 1.5 | 73 |
| 44 | Electron Mobility via Polaron Hopping in Bulk Ceria: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 14502-14509. | 1.5 | 75 |
| 45 | Importance of the Metalâ€“Oxide Interface in Catalysis: In Situ Studies of the Waterâ€“Gas Shift Reaction by Ambientâ€Pressure Xâ€ray Photoelectron Spectroscopy. Angewandte Chemie - International Edition, 2013, 52, 5101-5105. | 7.2 | 280 |
| 46 | Nanosized CoO Films on the Î±-Al<sub>2</sub>O<sub>3</sub> (0001) Surface: A Density Functional Study. Journal of Physical Chemistry C, 2013, 117, 22714-22722. | 1.5 | 6 |
| 47 | Role of the Siâ€“Si bond stability in the first stages of Ti diffusion on a Si(111) 2Ã—1 surface. A periodic DFT study. Applied Surface Science, 2013, 273, 496-501. | 3.1 | 2 |
| 48 | Transport Properties in the CeO<sub>2â€“x</sub>(111) Surface: From Charge Distribution to Ion-Electron Collaborative Migration. Journal of Physical Chemistry C, 2013, 117, 25497-25503. | 1.5 | 41 |
| 49 | Effect of dispersion correction on the Au(1 1 1)-H2O interface: A first-principles study. Journal of Chemical Physics, 2012, 137, 114709. | 1.2 | 49 |
| 50 | Making Photo-selective TiO<sub>2</sub> Materials by Cationâ€“Anion Codoping: From Structure and Electronic Properties to Photoactivity. Journal of Physical Chemistry C, 2012, 116, 18759-18767. | 1.5 | 29 |
| 51 | Ceria(100) Nanotubes with Negative Strain Energy: A First-Principles Prediction. Journal of Physical Chemistry Letters, 2012, 3, 2092-2096. | 2.1 | 5 |
| 52 | Study of the TiSi interface formed by Ti deposition on a clean Si (100) surface. Surface Science, 2012, 606, 754-761. | 0.8 | 3 |
| 53 | Coumarin derivatives for dye sensitized solar cells: a TD-DFT study. Physical Chemistry Chemical Physics, 2012, 14, 225-233. | 1.3 | 193 |
| 54 | Molecular modification of coumarin dyes for more efficient dye sensitized solar cells. Journal of Chemical Physics, 2012, 136, 194702. | 1.2 | 36 |

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| 55 | Communication: Improving the density functional theory+U description of CeO2 by including the contribution of the O 2p electrons. Journal of Chemical Physics, 2012, 136, 041101. | 1.2 | 62 |
| 56 | First-principles molecular dynamics simulations of the H2O / Cu(111) interface. Journal of Molecular Modeling, 2012, 18, 2433-2442. | 0.8 | 17 |
| 57 | Nitrogen/gold codoping of the TiO2(101) anatase surface. A theoretical study based on DFT calculations. Physical Chemistry Chemical Physics, 2011, 13, 11340. | 1.3 | 38 |
| 58 | CO Oxidation on Inverse CeO<sub>x</sub>/Cu(111) Catalysts: High Catalytic Activity and Ceria-Promoted Dissociation of O<sub>2</sub>. Journal of the American Chemical Society, 2011, 133, 3444-3451. | 6.6 | 241 |
| 59 | Understanding Acetaldehyde Thermal Chemistry on the TiO<sub>2</sub> (110) Rutile Surface: From Adsorption to Reactivity. Journal of Physical Chemistry C, 2011, 115, 2819-2825. | 1.5 | 22 |
| 60 | Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO<sub>2</sub>and Ce<sub>2</sub>O<sub>3</sub>. Journal of Chemical Theory and Computation, 2011, 7, 56-65. | 2.3 | 125 |
| 61 | Structural Defects in W-Doped TiO<sub>2</sub> (101) Anatase Surface: Density Functional Study. Journal of Physical Chemistry C, 2011, 115, 16970-16976. | 1.5 | 34 |
| 62 | Direct vs Indirect Mechanisms for Electron Injection in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2011, 115, 11293-11301. | 1.5 | 129 |
| 63 | Electronic structure and optical spectra of catechol on TiO<sub>2</sub>nanoparticles from real time TD-DFT simulations. Physical Chemistry Chemical Physics, 2011, 13, 1506-1514. | 1.3 | 103 |
| 64 | Direct vs. indirect mechanisms for electron injection in DSSC: Catechol and alizarin. Computational and Theoretical Chemistry, 2011, 975, 99-105. | 1.1 | 49 |
| 65 | Coverage and charge dependent adsorption of butanethiol on the Au(111) surface: A density functional theory study. Computational and Theoretical Chemistry, 2011, 975, 116-121. | 1.1 | 10 |
| 66 | Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity. Topics in Catalysis, 2011, 54, 219-228. | 1.3 | 25 |
| 67 | Determining the Behavior of RuO<sub>x</sub> Nanoparticles in Mixedâ€Metal Oxides: Structural and Catalytic Properties of RuO<sub>2</sub>/TiO<sub>2</sub>(110) Surfaces. Angewandte Chemie - International Edition, 2011, 50, 10198-10202. | 7.2 | 48 |
| 68 | Thiodiacetateâ€“Manganese Chemistry with N ligands: Unique Control of the Supramolecular Arrangement over the Metal Coordination Mode. Chemistry - A European Journal, 2011, 17, 10600-10617. | 1.7 | 29 |
| 69 | Real-Time TD-DFT Simulations in Dye Sensitized Solar Cells: The Electronic Absorption Spectrum of Alizarin Supported on TiO<sub>2</sub> Nanoclusters. Journal of Chemical Theory and Computation, 2010, 6, 2856-2865. | 2.3 | 170 |
| 70 | Charge state of metal atoms on oxide supports: a systematic study based on simulated infrared spectroscopy and density functional theory. Theoretical Chemistry Accounts, 2010, 126, 265-273. | 0.5 | 17 |
| 71 | Effect of interface structure on the Ru on HfO2 work function. Journal of Materials Science, 2010, 45, 4924-4928. | 1.7 | 2 |
| 72 | Gold, Copper, and Platinum Nanoparticles Dispersed on CeO<sub>x</sub>/TiO<sub>2</sub>(110) Surfaces: High Water-Gas Shift Activity and the Nature of the Mixed-Metal Oxide at the Nanometer Level. Journal of the American Chemical Society, 2010, 132, 356-363. | 6.6 | 247 |

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| 73 | A theoretical insight into the catalytic effect of a mixed-metal oxide at the nanometer level: The case of the highly active metal/CeOx/TiO2(110) catalysts. Journal of Chemical Physics, 2010, 132, 104703. | 1.2 | 93 |
| 74 | Density Functional Theory Study of the Interaction of Cu, Ag, and Au Atoms with the Regular CeO<sub>2</sub>(111) Surface. Journal of Physical Chemistry C, 2010, 114, 1934-1941. | 1.5 | 108 |
| 75 | First-principles study of ionic oxygen mobility of Sr-containing LaAlO<sub>3</sub>perovskite. Journal of Physics Condensed Matter, 2009, 21, 305502. | 0.7 | 2 |
| 76 | High catalytic activity of Au/CeO <sub>x</sub> /TiO <sub>2</sub> (110) controlled by the nature of the mixed-metal oxide at the nanometer level. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4975-4980. | 3.3 | 257 |
| 77 | Waterâ€Gas Shift Reaction on a Highly Active Inverse CeO<sub>x</sub>/Cu(111) Catalyst: Unique Role of Ceria Nanoparticles. Angewandte Chemie - International Edition, 2009, 48, 8047-8050. | 7.2 | 262 |
| 78 | High Waterâ^'Gas Shift Activity in TiO<sub>2</sub>(110) Supported Cu and Au Nanoparticles: Role of the Oxide and Metal Particle Size. Journal of Physical Chemistry C, 2009, 113, 7364-7370. | 1.5 | 223 |
| 79 | Ca Deposition on TiO<sub>2</sub>(110) Surfaces: Insights from Quantum Calculations. Journal of Physical Chemistry C, 2009, 113, 3740-3745. | 1.5 | 7 |
| 80 | A Density Functional Study of Initial Steps in the Oxidation of Early Transition Metal Nitrides, MN (M =) Tj ETQq0 0 0 rgBT /Overlock 10 T | 1.5 | 12 |
| 81 | Carbon Doping of the TiO<sub>2</sub> (110) Rutile Surface. A Theoretical Study Based on DFT. Chemistry of Materials, 2009, 21, 1431-1438. | 3.2 | 39 |
| 82 | Redox properties of gold-substituted zirconia surfaces. Journal of Materials Chemistry, 2009, 19, 710-717. | 6.7 | 12 |
| 83 | Role of Coverage and Surface Oxidation Degree in the Adsorption of Acetone on TiO<sub>2</sub>(110). A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 19973-19980. | 1.5 | 24 |
| 84 | On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO[sub 2](111). Journal of Chemical Physics, 2009, 131, 094702. | 1.2 | 64 |
| 85 | Electronic charge transfer between ceria surfaces and gold adatoms: a GGA+U investigation. Physical Chemistry Chemical Physics, 2009, 11, 5246. | 1.3 | 83 |
| 86 | Changing the physical and chemical properties of titanium oxynitrides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiN</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:m changing the composition. Physical Review B, 2009, 80, . | 1.1 | 48 |
| 87 | Methanol and Water Dissociation on TiO2 (110): The Role of Surface Oxygen. Journal of Physical Chemistry C, 2008, 112, 17737-17740. | 1.5 | 92 |
| 88 | N Doping of Rutile TiO<sub>2</sub> (110) Surface. A Theoretical DFT Study. Journal of Physical Chemistry C, 2008, 112, 2624-2631. | 1.5 | 107 |
| 89 | Atomic Layer Deposition of Hafnium Oxide from Hafnium Chloride and Water. Journal of the American Chemical Society, 2008, 130, 11996-12006. | 6.6 | 45 |
| 90 | Au â†" N Synergy and N-Doping of Metal Oxide-Based Photocatalysts. Journal of the American Chemical Society, 2008, 130, 12056-12063. | 6.6 | 115 |

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| 91 | Effect of on-site Coulomb repulsion term<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>on the band-gap states of the reduced rutile (110)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>surface. | 1.1 | 165 |
| 92 | Interaction of oxygen with TiN(001):Nâ†"O exchange and oxidation process. Journal of Chemical Physics, 2007, 126, 244713. | 1.2 | 51 |
| 93 | Influence of Temperature on the Interaction between Pd Clusters and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>(110) Surface. Physical Review Letters, 2007, 99, 066102. | 2.9 | 11 |
| 94 | Adsorption of Pd Atoms and Dimers on the TiO2(110) Surface:â€‰ A First Principles Study. Journal of Physical Chemistry C, 2007, 111, 3949-3955. | 1.5 | 51 |
| 95 | Theoretical Investigation of the Deposition of Cu, Ag, and Au Atoms on the ZrO2(111) Surface. Journal of Physical Chemistry C, 2007, 111, 10448-10454. | 1.5 | 58 |
| 96 | First-Principles Investigation of the Structure, Energetics, and Electronic Properties of Ru/HfO2Interfaces. Journal of Physical Chemistry C, 2007, 111, 9203-9210. | 1.5 | 11 |
| 97 | Methanol Adsorption and Dissociation on TiO2(110) from First Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 10023-10028. | 1.5 | 106 |
| 98 | Classical molecular dynamics simulations of gold clusters deposited on rutile TiO2(110) surface. Catalysis Today, 2007, 128, 230-234. | 2.2 | 4 |
| 99 | First-Principles Investigation of Hydroxylated Monoclinic HfO2 Surfaces. Chemistry of Materials, 2006, 18, 3397-3403. | 3.2 | 30 |
| 100 | First-principles calculations of structural and electronic properties of monoclinic hafnia surfaces. Physical Review B, 2006, 73, . | 1.1 | 71 |
| 101 | Unravelling the Origin of the High-Catalytic Activity of Supported Au:Â A Density-Functional Theory-Based Interpretation. Journal of the American Chemical Society, 2006, 128, 15600-15601. | 6.6 | 65 |
| 102 | V@Au12-:Â An Improved Novel Catalyst for CO Oxidation?. Journal of Physical Chemistry B, 2006, 110, 11600-11603. | 1.2 | 61 |
| 103 | Ba Adsorption on the Stoichiometric and Defective TiO2 (110) Surface from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 19552-19556. | 1.2 | 5 |
| 104 | From periodic DFT calculations to classical molecular dynamics simulations. Computational Materials Science, 2006, 35, 183-186. | 1.4 | 8 |
| 105 | Ba adsorption on the TiO2 (110) surface. A density functional study. Computational and Theoretical Chemistry, 2006, 769, 237-242. | 1.5 | 4 |
| 106 | Structure and Dynamics of Methyl-substituted Beryllocene: [Be(C5Me5)2]. Theoretical Chemistry Accounts, 2006, 116, 480-485. | 0.5 | 6 |
| 107 | Proposal for a modified MÃ¸ller-Plesset perturbation theory. Physical Review A, 2006, 73, . | 1.0 | 3 |
| 108 | The constrained space orbital variation analysis for periodic ab initio calculations. Journal of Chemical Physics, 2006, 124, 194105. | 1.2 | 7 |

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| 109 | N doping of TiO2(110): Photoemission and density-functional studies. Journal of Chemical Physics, 2006, 125, 094706. | 1.2 | 127 |
| 110 | Cu, Ag and Au atoms deposited on the Î±-Al2O3(0001) surface: a comparative density functional study. Surface Science, 2005, 575, 189-196. | 0.8 | 63 |
| 111 | Supramolecular Interactions as Determining Factors of the Geometry of Metallic Building Blocks: Tetracarboxylate Dimanganese Species. Angewandte Chemie - International Edition, 2005, 44, 3429-3432. | 7.2 | 27 |
| 112 | Interaction potentials from periodic density-functional theory calculations: Molecular-dynamics simulations of Au clusters deposited on the TiN (001) surface. Journal of Chemical Physics, 2005, 123, 244706. | 1.2 | 9 |
| 113 | Mechanism of Cu Deposition on theÎ±â^'Al2O3(0001) Surface. Physical Review Letters, 2005, 94, 016104. | 2.9 | 37 |
| 114 | N2O Decomposition on TiO2 (110) from Dynamic First-Principles Calculations. Journal of Physical Chemistry B, 2005, 109, 16223-16226. | 1.2 | 38 |
| 115 | Role of vacancies in the structural stability ofÎ±â^'TiO: A first-principles study based on density-functional calculations. Physical Review B, 2005, 72, . | 1.1 | 50 |
| 116 | Atomistic simulations of Cu deposition on the Î±-Al2O3 (0001) surface. Computational and Theoretical Chemistry, 2004, 709, 79-85. | 1.5 | 1 |
| 117 | First principles simulations of Cu and Au deposition on Î±-Al2O3 (0001) surface. Applied Surface Science, 2004, 238, 228-232. | 3.1 | 19 |
| 118 | Adsorption of Pd atoms on Î³-Al2O3: a density functional study of metalâ€“support interactions. Applied Surface Science, 2004, 238, 82-85. | 3.1 | 23 |
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| 120 | Density Functional Theory Study of Co, Rh, and Ir Atoms Deposited on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2004, 108, 15671-15678. | 1.2 | 30 |
| 121 | Synthesis, Solid-State Structure, and Bonding Analysis of the Beryllocenes[Be(C5Me4H)2],[Be(C5Me5)2], and[Be(C5Me5)(C5Me4H)]. Chemistry - A European Journal, 2003, 9, 4452-4461. | 1.7 | 37 |
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| 123 | A parametrical embedding method for catalytic modeling. Journal of Molecular Catalysis A, 2003, 191, 101-112. | 4.8 | 3 |
| 124 | Surface model and exchange-correlation functional effects on the description of Pd/Î±-Al2O3(0001). Journal of Chemical Physics, 2002, 116, 1684-1691. | 1.2 | 51 |
| 125 | Interaction of Pd withÎ±â^'Al2O3(0001):â€ƒA case study of modeling the metal-oxide interface on complex substrates. Physical Review B, 2002, 65, . | 1.1 | 55 |
| 126 | First Principles Study of Cu Atoms Deposited on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2002, 106, 11495-11500. | 1.2 | 34 |

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| 127 | Molecular Dynamics Simulations of Pd Deposition on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2001, 105, 12111-12117. | 1.2 | 30 |
| 128 | Cu, Ag, and Au atoms adsorbed on TiO2(110): cluster and periodic calculations. Surface Science, 2001, 471, 21-31. | 0.8 | 131 |
| 129 | Theoretical Approach to Ionic Conductivity in PhosphorusOxynitride Compounds. Journal of Solid State Chemistry, 2001, 161, 73-79. | 1.4 | 12 |
| 130 | DFTversus CI determination of the electron-transfer matrix element in some case examples. International Journal of Quantum Chemistry, 2000, 76, 458-463. | 1.0 | 12 |
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| 135 | Theoretical investigations of NMR chemical shieldings on the AlPON catalyst system. Journal of Non-Crystalline Solids, 2000, 263-264, 189-194. | 1.5 | 7 |
| 136 | Accurate ab initio determination of magnetic interactions and hopping integrals in La2â^'xSrxCuO4 systems. Journal of Chemical Physics, 2000, 112, 5158-5167. | 1.2 | 85 |
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| 138 | A periodic Hartreeâ€“Fock study of Na adsorption on the TiO2(110) rutile surface. Chemical Physics Letters, 1999, 303, 111-116. | 1.2 | 18 |
| 139 | Ab initio systematic determination of the tâ€“J effective Hamiltonian parameters for superconducting Cu-oxides. Chemical Physics Letters, 1999, 307, 102-108. | 1.2 | 47 |
| 140 | Adsorption Energetics of NO and CO on Pt(111). Journal of Cluster Science, 1999, 10, 581-590. | 1.7 | 6 |
| 141 | Cr2O3 (0001) oxygen-terminating surface. A molecular dynamics study. Computational and Theoretical Chemistry, 1999, 463, 185-190. | 1.5 | 13 |
| 142 | Ab initio compact group model potentials for describing environment effects in cluster calculations. Journal of Computational Chemistry, 1999, 20, 1145-1152. | 1.5 | 7 |
| 143 | Adsorption of Acetone onto MgO: Experimental and Theoretical Evidence for the Presence of a Surface Enolate. Angewandte Chemie - International Edition, 1999, 38, 506-509. | 7.2 | 24 |
| 144 | Synthesis, Structural Characterization, and MO Calculations of Vanadium Imido Complexes Containing Bidentate Phosphine Coligands. Inorganic Chemistry, 1999, 38, 4462-4466. | 1.9 | 17 |

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