# Notker RÃ¶sch

List of Publications by Year
in descending order



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|---|---|---|---|
| 177 papers | 6,781 citations | 50244 46 h-index | 74108 75 g-index |
| 181 all docs | 181 docs citations | 181 times ranked | 5423 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Ethene Conversion at a Zeoliteâ€Supported Ir(I) Complex. A Computational Perspective on a Singleâ€Site Catalyst System. ChemCatChem, 2021, 13, 3421-3433. | 1.8 | 2 |
| 2 | Probing the Positions of TeO Moieties in the Channels of the MoVNbTeO M1 Catalyst: A Density Functional Theory Model Study. Catalysis Letters, 2021, 151, 2884-2893. | 1.4 | 4 |
| 3 | The origin of the particle-size-dependent selectivity in 1-butene isomerization and hydrogenation on Pd/Al2O3 catalysts. Nature Communications, 2021, 12, 6098. | 5.8 | 16 |
| 4 | Configurations of V4+ centers in the MoVO catalyst material. A systematic stability analysis of DFT results. SN Applied Sciences, 2020, 2, 1. | 1.5 | 0 |
| 5 | How TeO Defects in the MoVNbTeO Catalyst Material Affect the V<sup>4+</sup> Distribution: A Computational Study. Journal of Physical Chemistry C, 2020, 124, 18628-18638. | 1.5 | 5 |
| 6 | Strain and Low-Coordination Effects on Monolayer Nanoislands of Pd and Pt on Au(111): A Comparative Analysis Based on Density Functional Results. Journal of Physical Chemistry C, 2020, 124, 13225-13230. | 1.5 | 9 |
| 7 | Modeling the effect of ligands and solvation on hydrolysis variants in the Pd(II)-Catalyzed hydroxycarbonylation of pentenoic acids. Journal of Organometallic Chemistry, 2020, 914, 121221. | 0.8 | 0 |
| 8 | Hydration Structure and Hydrolysis of U(IV) and Np(IV) Ions: A Comparative Density Functional Study Using a Modified Continuum Solvation Approach. Journal of Physical Chemistry A, 2020, 124, 3805-3814. | 1.1 | 3 |
| 9 | Mononuclear Hydroxo Carbonato Complexes of Np(V), Np(VI), and U(VI): A Density Functional Study. European Journal of Inorganic Chemistry, 2019, 2019, 4516-4526. | 1.0 | 2 |
| 10 | Câ€“C coupling at a zeolite-supported Rh(<scp>i</scp>) complex. DFT search for the mechanism. Catalysis Science and Technology, 2019, 9, 2781-2793. | 2.1 | 8 |
| 11 | Interdisciplinary Round-Robin Test on Molecular Spectroscopy of the U(VI) Acetate System. ACS Omega, 2019, 4, 8167-8177. | 1.6 | 5 |
| 12 | Reactivity trends of the MoVO<sub>x</sub>mixed metal oxide catalyst from density functional modeling. Catalysis Science and Technology, 2019, 9, 1559-1569. | 2.1 | 10 |
| 13 | CO2 reduction by H2 to CHO on Ru(0001): DFT evaluation of three pathways. Surface Science, 2019, 681, 54-58. | 0.8 | 11 |
| 14 | Ethanol Conversion to Ethylene and Acetaldehyde over Rhodium(I) Exchanged Faujasite Zeolite. A QM/MM and Microkinetic Study. Journal of Physical Chemistry C, 2018, 122, 2783-2795. | 1.5 | 8 |
| 15 | Modeling Polaron-Coupled Li Cation Diffusion in V<sub>2</sub>O<sub>5</sub> Cathode Material. Journal of Physical Chemistry C, 2018, 122, 150-157. | 1.5 | 26 |
| 16 | How the distribution of reduced vanadium centers affects structure and stability of the MoVO<sub>x</sub>material. Catalysis Science and Technology, 2018, 8, 2654-2660. | 2.1 | 9 |
| 17 | Ethene Dimerization and Hydrogenation over a Zeolite-Supported Rh(I)-Carbonyl Complex: Mechanistic Insights from DFT Modeling. ACS Catalysis, 2018, 8, 9836-9846. | 5.5 | 14 |
| 18 | Catalytic Transformations of 1-Butene over Palladium. A Combined Experimental and Theoretical Study. ACS Catalysis, 2018, 8, 5675-5685. | 5.5 | 14 |

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| 19 | Acrolein oxidation to acrylic acid over the MoVOx material. Insights from DFT modeling. Applied Catalysis A: General, 2018, 565, 68-75. | 2.2 | 13 |
| 20 | DFT Variants for Mixed-Metal Oxides. Benchmarks Using Multi-Center Cluster Models. Journal of Physical Chemistry A, 2018, 122, 7042-7050. | 1.1 | 9 |
| 21 | Modeling the Effect of the Electrolyte on Standard Reduction Potentials of Polyoxometalates. Journal of Physical Chemistry C, 2018, 122, 18545-18553. | 1.5 | 3 |
| 22 | Quantum chemical modeling of tri-Mn-substituted W-based Keggin polyoxoanions. Electrochimica Acta, 2017, 231, 659-669. | 2.6 | 8 |
| 23 | Evaluation of density functionals for elementary steps of selective oxidation reactions. Computational and Theoretical Chemistry, 2017, 1101, 36-45. | 1.1 | 11 |
| 24 | Ethene hydrogenation vs. dimerization over a faujasite-supported [Rh(C<sub>2</sub>H<sub>4</sub>)<sub>2</sub>] complex. A computational study of mechanism. Catalysis Science and Technology, 2017, 7, 102-113. | 2.1 | 18 |
| 25 | Crystal-Chemical Composition of Dicoctahedral Smectites: An Energy-Based Assessment of Empirical Relations. ACS Earth and Space Chemistry, 2017, 1, 629-636. | 1.2 | 6 |
| 26 | Surface Reactivity of the Vanadium Phosphate Catalyst for the Oxidation of Methane. Topics in Catalysis, 2017, 60, 1698-1708. | 1.3 | 4 |
| 27 | Palladium-Catalyzed Hydroxycarbonylation of Pentenoic Acids. Computational and Experimental Studies on the Catalytic Selectivity. ACS Catalysis, 2017, 7, 7070-7080. | 5.5 | 27 |
| 28 | Size-Dependence of the Adsorption Energy of CO on Pt Nanoparticles: Tracing Two Intersecting Trends by DFT Calculations. Journal of Physical Chemistry C, 2017, 121, 17371-17377. | 1.5 | 39 |
| 29 | Identification of surface species by vibrational normal mode analysis. A DFT study. Surface Science, 2017, 664, 233-240. | 0.8 | 1 |
| 30 | Carboxylic acid formation by hydroxyl insertion into acyl moieties on late transition metals. Catalysis Science and Technology, 2017, 7, 5365-5375. | 2.1 | 2 |
| 31 | Transformations of Organic Molecules over Metal Surfaces: Insights from Computational Catalysis. Chemical Record, 2016, 16, 2388-2404. | 2.9 | 14 |
| 32 | Toward a Reliable Energetics of Adsorption at Solvated Mineral Surfaces: A Computational Study of Uranyl(VI) on 2:1 Clay Minerals. Journal of Physical Chemistry C, 2016, 120, 324-335. | 1.5 | 18 |
| 33 | Extending the cluster scaling technique to ruthenium clusters with hcp structures. Surface Science, 2016, 643, 156-163. | 0.8 | 10 |
| 34 | Three-dimensional reference interaction site model solvent combined with a quantum mechanical treatment of the solute. Computational and Theoretical Chemistry, 2015, 1070, 143-151. | 1.1 | 5 |
| 35 | Hydrogen Adsorption on Small Zeolite-Supported Rhodium Clusters. A Density Functional Study. Journal of Physical Chemistry C, 2015, 119, 1121-1129. | 1.5 | 13 |
| 36 | Structure and electronic properties of MoVO type mixed-metal oxides â€“ a combined view by experiment and theory. Dalton Transactions, 2015, 44, 13778-13795. | 1.6 | 21 |

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| 37 | Uranyl Solvation by a Three-Dimensional Reference Interaction Site Model. Journal of Physical Chemistry A, 2015, 119, 8702-8713. | 1.1 | 2 |
| 38 | Assessment of Hybrid Density Functionals for the Adsorption of Carbon Monoxide on Platinum Model Clusters. Journal of Physical Chemistry A, 2015, 119, 4051-4056. | 1.1 | 16 |
| 39 | Câ€“O cleavage of aromatic oxygenates over ruthenium catalysts. A computational study of reactions at step sites. Physical Chemistry Chemical Physics, 2015, 17, 15324-15330. | 1.3 | 26 |
| 40 | Size-dependent properties of transition metal clusters: from molecules to crystals and surfaces â€“ computational studies with the program ParaGauss. Physical Chemistry Chemical Physics, 2015, 17, 28463-28483. | 1.3 | 16 |
| 41 | Uranyl solvation by a reference interaction site model. Computational and Theoretical Chemistry, 2015, 1051, 151-160. | 1.1 | 5 |
| 42 | Comment on â€œFirst-principles-based embedded atom method for PdAu nanoparticlesâ€• Physical Review B, 2014, 89, . | 1.1 | 3 |
| 43 | Interaction of silica-supported small silver clusters with molecular oxygen. A computational study. Surface Science, 2014, 630, 265-272. | 0.8 | 12 |
| 44 | The DFT+Umol method and its application to the adsorption of CO on platinum model clusters. Journal of Chemical Physics, 2014, 140, 174709. | 1.2 | 10 |
| 45 | Predicting adsorption enthalpies on silicalite and HZSMâ€5: A benchmark study on DFT strategies addressing dispersion interactions. Journal of Computational Chemistry, 2014, 35, 809-819. | 1.5 | 31 |
| 46 | Hydrodeoxygenation of Guaiacol over Ru(0001): A DFT Study. ACS Catalysis, 2014, 4, 4178-4188. | 5.5 | 105 |
| 47 | Load balancing by workâ€“stealing in quantum chemistry calculations: Application to hybrid density functional methods. International Journal of Quantum Chemistry, 2014, 114, 813-822. | 1.0 | 9 |
| 48 | Modeling Catalytic Steps on Extra-Framework Metal Centers in Zeolites. A Case Study on Ethylene Dimerization. Journal of Physical Chemistry C, 2014, 118, 25077-25088. | 1.5 | 16 |
| 49 | DFT cluster model study of MoVO-type mixed-metal oxides. Computational and Theoretical Chemistry, 2014, 1045, 57-65. | 1.1 | 7 |
| 50 | Monolayer Nanoislands of Pt on Au and Cu: A First-Principles Computational Study. Journal of Physical Chemistry C, 2014, 118, 22102-22110. | 1.5 | 8 |
| 51 | Hybrid Density Functionals for Clusters of Late Transition Metals: Assessing Energetic and Structural Properties. Journal of Chemical Theory and Computation, 2014, 10, 4408-4416. | 2.3 | 21 |
| 52 | A DFTÂ+ÂUmol model study of the self-interaction error in standard density functional calculations of Ni(CO) m (mÂ=Â1â€“4). Theoretical Chemistry Accounts, 2014, 133, . | 0.5 | 2 |
| 53 | Formation of CO<sub>2</sub> and Ethane from Propionyl over Platinum: A Density Functional Theory Study. ACS Catalysis, 2013, 3, 1730-1738. | 5.5 | 5 |
| 54 | Scalable properties of metal clusters: A comparative DFT study of ionic-core treatments. Chemical Physics Letters, 2013, 578, 92-96. | 1.2 | 8 |

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| 55 | Metalâ€Free Polymerization of Phenylsilane: Tris(pentafluorophenyl)boraneâ€Catalyzed Synthesis of Branched Polysilanes at Elevated Temperatures. Chemistry - A European Journal, 2013, 19, 12526-12536. | 1.7 | 28 |
| 56 | Decomposition of Ethanol Over Ru(0001): A DFT Study. Topics in Catalysis, 2013, 56, 874-884. | 1.3 | 36 |
| 57 | Structure of Pd/Au Alloy Nanoparticles from a Density Functional Theory-Based Embedded-Atom Potential. Journal of Physical Chemistry C, 2013, 117, 21810-21822. | 1.5 | 22 |
| 58 | Formation of n-hexane from methylcyclopentane via a metallacyclobutane intermediate at step sites of Pt surfaces: Mechanism from first-principles calculations. Journal of Catalysis, 2013, 299, 146-149. | 3.1 | 10 |
| 59 | Efficient Two-Step Procedures for Locating Transition States of Surface Reactions. Journal of Chemical Theory and Computation, 2013, 9, 588-599. | 2.3 | 7 |
| 60 | Activation of Hydrogen Peroxide by Ionic Liquids: Mechanistic Studies and Application in the Epoxidation of Olefins. Chemistry - A European Journal, 2013, 19, 5972-5979. | 1.7 | 47 |
| 61 | Ring-Opening Reactions of Methylcyclopentane over Metal Catalysts, M = Pt, Rh, Ir, and Pd: A Mechanistic Study from First-Principles Calculations. ACS Catalysis, 2013, 3, 196-205. | 5.5 | 33 |
| 62 | Formation of Propane in the Aqueousâ€Phase Processing of 1â€Propanol over Platinum: A DFT Study. ChemCatChem, 2013, 5, 3299-3308. | 1.8 | 10 |
| 63 | Carbon Dioxide Insertion into Diamines: A Computational Study of Solvent Effects. ChemSusChem, 2012, 5, 1967-1973. | 3.6 | 11 |
| 64 | Theoretical study on the leaching of palladium in a CO atmosphere. Catalysis Science and Technology, 2012, 2, 2238. | 2.1 | 18 |
| 65 | Reverse hydrogen spillover on and hydrogenation of supported metal clusters: insights from computational model studies. Physical Chemistry Chemical Physics, 2012, 14, 5879. | 1.3 | 18 |
| 66 | Hydrogen adsorption on and spillover from Au- and Cu-supported Pt3 and Pd3 clusters: a density functional study. Physical Chemistry Chemical Physics, 2012, 14, 16062. | 1.3 | 28 |
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| 68 | Metal-Supported Metal Clusters: A Density Functional Study of Pt<sub>3</sub> and Pd<sub>3</sub>. Journal of Physical Chemistry C, 2012, 116, 10057-10063. | 1.5 | 12 |
| 69 | Scalable properties of metal clusters: A comparative study of modern exchange-correlation functionals. Journal of Chemical Physics, 2012, 137, 034102. | 1.2 | 20 |
| 70 | Size Dependence of the Adsorption Energy of CO on Metal Nanoparticles: A DFT Search for the Minimum Value. Nano Letters, 2012, 12, 2134-2139. | 4.5 | 155 |
| 71 | Structureâ€Dependence of the magnetic moment in small palladium clusters: Surprising results from the M06â€L Metaâ€GGA functional. International Journal of Quantum Chemistry, 2012, 112, 113-120. | 1.0 | 10 |
| 72 | Cationic Zinc Species in ZSM-5 Zeolites: Structure and Stability from Embedded Cluster Modeling. Soft Materials, 2012, 10, 216-234. | 0.8 | 3 |

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| 73 | Uranyl(VI) Complexation by Sulfonate Ligands: A Relativistic Density Functional and Timeâ€Resolved Laserâ€Induced Fluorescence Spectroscopy Study. European Journal of Inorganic Chemistry, 2012, 2012, 3636-3644. | 1.0 | 7 |
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| 77 | Comment on â€œTowards understanding the bifunctional hydrodeoxygenation and aqueous phase reforming of glycerolâ€•[J. Catal. 269 (2010) 411â€“420]. Journal of Catalysis, 2012, 287, 210-213. | 3.1 | 13 |
| 78 | DFT Studies of Palladium Model Catalysts: Structure and Size Effects. Journal of Cluster Science, 2011, 22, 433-448. | 1.7 | 39 |
| 79 | Impurity Atoms on Small Transition Metal Clusters. Insights from Density Functional Model Studies. Topics in Catalysis, 2011, 54, 363-377. | 1.3 | 8 |
| 80 | Self-interaction artifacts on structural features of uranyl monohydroxide from Kohnâ€“Sham calculations. Theoretical Chemistry Accounts, 2011, 130, 361-369. | 0.5 | 5 |
| 81 | Uranyl complexation by monodentate nitrogen donor ligands. A relativistic density functional study. International Journal of Quantum Chemistry, 2011, 111, 2045-2053. | 1.0 | 4 |
| 82 | Effects of the self-interaction error in Kohnâ€“Sham calculations: A DFT+U case study on penta-aqua uranyl(VI). Computational and Theoretical Chemistry, 2011, 963, 337-343. | 1.1 | 12 |
| 83 | Decomposition of ethylene on transition metal surfaces M(111). A comparative DFT study of model reactions for M=Pd, Pt, Rh, Ni. Journal of Molecular Catalysis A, 2011, 344, 37-46. | 4.8 | 52 |
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| 86 | Small gold species at hydroxylated alumina surfaces. A computational study using embedded-cluster models of Î±-Al2O3(0001). Chemical Physics Letters, 2010, 494, 243-248. | 1.2 | 3 |
| 87 | Small gold species supported on alumina. A computational study of Î±â€Al<sub>2</sub>O<sub>3</sub>(0001) and Î³â€Al<sub>2</sub>O<sub>3</sub>(001) using an embeddedâ€cluster approach. Physica Status Solidi (B): Basic Research, 2010, 247, 1023-1031. | 0.7 | 10 |
| 88 | Variational fitting methods for electronic structure calculations. Molecular Physics, 2010, 108, 3167-3180. | 0.8 | 89 |
| 89 | Comparative density functional study of the complexes [UO2(CO3)3]4â^' and [(UO2)3(CO3)6]6â^' in aqueous solution. Dalton Transactions, 2010, 39, 5705. | 1.6 | 15 |
| 90 | Transformations of Ethylene on the Pd(111) Surface: A Density Functional Study. Journal of Physical Chemistry C, 2010, 114, 17683-17692. | 1.5 | 47 |

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| 91 | Ethylidyne Formation from Ethylene over Pt(111): A Mechanistic Study from First-Principle Calculations. Journal of Physical Chemistry C, 2010, 114, 12190-12201. | 1.5 | 77 |
| 92 | Saturation of Small Supported Metal Clusters by Adsorbed Hydrogen. A Computational Study on Tetrahedral Models of Rh<sub>4</sub>, Ir<sub>4</sub>, and Pt<sub>4</sub>. Journal of Physical Chemistry C, 2010, 114, 8500-8506. | 1.5 | 27 |
| 93 | Redox behavior of small metal clusters with respect to hydrogen. The effect of the cluster charge from density functional results. Physical Chemistry Chemical Physics, 2010, 12, 11015. | 1.3 | 6 |
| 94 | Particle-size dependent heats of adsorption of CO on supported Pd nanoparticles as measured with a single-crystal microcalorimeter. Physical Review B, 2010, 81, . | 1.1 | 77 |
| 95 | Role of aliphatic and phenolic hydroxyl groups in uranyl complexation by humic substances. Inorganica Chimica Acta, 2009, 362, 2542-2550. | 1.2 | 14 |
| 96 | The DFT+U method in the linear combination of Gaussian-type orbitals framework: Role of 4f orbitals in the bonding of LuF3. Chemical Physics Letters, 2009, 468, 158-161. | 1.2 | 20 |
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| 98 | Ethylene Conversion to Ethylidyne over Pd(111): Revisiting the Mechanism with First-Principles Calculations. Journal of Physical Chemistry C, 2009, 113, 2512-2520. | 1.5 | 56 |
| 99 | Theoretical study of carbon species on Pd(111): competition between migration of C atoms to the subsurface interlayer and formation of Cn clusters on the surface. Physical Chemistry Chemical Physics, 2009, 11, 10955. | 1.3 | 27 |
| 100 | Ethylidyne Formation from Ethylene over Pd(111): Alternative Routes from a Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 15373-15379. | 1.5 | 29 |
| 101 | Uranyl monocarboxylates of aromatic acids: A density functional model study of uranyl humate complexation. Dalton Transactions, 2009, , 3590. | 1.6 | 22 |
| 102 | Electronic and Geometric Structure of the Cluster Compound Au<sub>55</sub>[P(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>]<sub>12</sub>C<sub>l</sub>6. A Computational Study. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2009, 64, 1246-1258. | 0.3 | 8 |
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| 104 | Size-Dependence of Adsorption Properties of Metal Nanoparticles: A Density Functional Study on Palladium Nanoclusters. Journal of Physical Chemistry C, 2008, 112, 20269-20275. | 1.5 | 86 |
| 105 | Hydrogen Activation on Silver:â€‰ A Computational Study on Surface and Subsurface Oxygen Species. Journal of Physical Chemistry C, 2008, 112, 1628-1635. | 1.5 | 44 |
| 106 | How the Câ”O Bond Breaks during Methanol Decomposition on Nanocrystallites of Palladium Catalysts. Journal of the American Chemical Society, 2008, 130, 9342-9352. | 6.6 | 77 |
| 107 | Hydrogen Adsorption on Zeolite-Supported Tetrairidium Clusters. Thermodynamic Modeling from Density Functional Calculations. Journal of Physical Chemistry C, 2008, 112, 18572-18577. | 1.5 | 18 |
| 108 | Atomic approximation to the projection on electronic states in the Douglas-Kroll-Hess approach to the relativistic Kohn-Sham method. Journal of Chemical Physics, 2008, 128, 244102. | 1.2 | 22 |

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| 109 | Impurity Effects on Small Pd Clusters: A Relativistic Density Functional Study of Pd4X, X = H, C, O. Journal of Physical Chemistry A, 2008, 112, 7739-7744. | 1.1 | 12 |
| 110 | CO Coordination at XNi<sub>4</sub>Clusters with Impurities X = H, C, O. A Density Functional Study. Journal of Physical Chemistry A, 2008, 112, 8523-8528. | 1.1 | 3 |
| 111 | Reverse Hydrogen Spillover onto Zeolite-Supported Metal Clusters:â€‰ An Embedded Cluster Density Functional Study of Models M<sub>6</sub>(M = Rh, Ir, or Au). Journal of Physical Chemistry C, 2007, 111, 12340-12351. | 1.5 | 57 |
| 112 | A computational study of H2dissociation on silver surfaces: The effect of oxygen in the added row structure of Ag(110). Physical Chemistry Chemical Physics, 2007, 9, 1247-1254. | 1.3 | 43 |
| 113 | Influence of Single Impurity Atoms on the Structure, Electronic, and Magnetic Properties of Ni5 Clusters. Journal of Physical Chemistry A, 2007, 111, 2067-2076. | 1.1 | 10 |
| 114 | Density Functional Study of Hydrogen Adsorption on Tetrairidium Supported on Hydroxylated and Dehydroxylated Zeolite Surfaces. Journal of Physical Chemistry C, 2007, 111, 14484-14492. | 1.5 | 25 |
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| 116 | Density Functional Embedded Cluster Study of Cu4, Ag4and Au4Species Interacting with Oxygen Vacancies on the MgO(001) Surface. Chemistry - A European Journal, 2007, 13, 277-286. | 1.7 | 22 |
| 117 | Modeling metal adsorption at amorphous silica: Gold atoms and dimers as example. Chemical Physics Letters, 2007, 444, 280-286. | 1.2 | 22 |
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| 120 | A Density Functional Study of Uranyl Monocarboxylates. Inorganic Chemistry, 2006, 45, 1480-1490. | 1.9 | 51 |
| 121 | Câ€“O bond scission of methoxide on Pd nanoparticles: A density functional study. Physical Chemistry Chemical Physics, 2006, 8, 2396-2401. | 1.3 | 24 |
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| 124 | Structure, stability, electronic and magnetic properties of Ni4 clusters containing impurity atoms. Physical Chemistry Chemical Physics, 2006, 8, 1282. | 1.3 | 21 |
| 125 | Systematic DFT Study of Gas Phase and Solvated Uranyl and Neptunyl Complexes [AnO2X4]n(An = U, Np;) Tj ETQq1 1 0.784314 rgBT | 1.9 | 41 |
| 126 | The IMOMM (Integrated Molecular Orbitals/Molecular Mechanics) Approach for Ligand-Stabilized Metal Clusters. Comparison to Full Density Functional Calculations for the Model Thiolate Cluster Cu13(SCH2CH3)8. Journal of Chemical Theory and Computation, 2006, 2, 47-58. | 2.3 | 11 |

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| 128 | Adsorption of acrolein on single-crystal surfaces of silver: Density functional studies. Chemical Physics Letters, 2006, 420, 60-64. | 1.2 | 25 |
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| 130 | The Heat of Formation of the Uranyl Dication: Theoretical Evaluation Based on Relativistic Density Functional Calculations. Chemistry - A European Journal, 2006, 12, 629-634. | 1.7 | 17 |
| 131 | Adsorption of carbon on Pd clusters of nanometer size: A first-principles theoretical study. Journal of Chemical Physics, 2005, 122, 174705. | 1.2 | 33 |
| 132 | The cluster Ir4 and its interaction with a hydrogen impurity. A density functional study. Physical Chemistry Chemical Physics, 2005, 7, 2656. | 1.3 | 36 |
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| 139 | Role of Solvation in the Reduction of the Uranyl Dication by Water:Â A Density Functional Study. Inorganic Chemistry, 2004, 43, 4080-4090. | 1.9 | 65 |
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| 142 | Density functional study of Pd nanoparticles with subsurface impurities of light element atoms. Physical Chemistry Chemical Physics, 2004, 6, 116-123. | 1.3 | 105 |
| 143 | Computational Study of Model Pdâ^'Zn Nanoclusters and Their Adsorption Complexes with CO Molecules. Journal of Physical Chemistry B, 2004, 108, 5424-5430. | 1.2 | 59 |
| 144 | Olefin Epoxidation with Inorganic Peroxides. Solutions to Four Long-Standing Controversies on the Mechanism of Oxygen Transfer. Accounts of Chemical Research, 2004, 37, 645-652. | 7.6 | 142 |

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