# Markus Pernpointner

List of Publications by Year
in descending order



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|---|---|---|---|
| 37 papers | 1,130 citations | 686830 13 h-index | 395343 33 g-index |
| 38 all docs | 38 docs citations | 38 times ranked | 1416 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | The DIRAC code for relativistic molecular calculations. Journal of Chemical Physics, 2020, 152, 204104. | 1.2 | 191 |
| 2 | Metal-Assisted Salphen Organic Frameworks (MaSOFs) with Trinuclear Metal Units for Synergic Gas Sorption. Chemistry of Materials, 2019, 31, 6210-6223. | 3.2 | 15 |
| 3 | Four-component relativistic calculations of electronic excitations in tris-(allyl)-iridium complex: Influence of spin-orbit coupling on the electronic structure and excitation spectrum. Chemical Physics, 2019, 523, 160-171. | 0.9 | 1 |
| 4 | Four-Component Polarization Propagator Calculations of Electron Excitations: Spectroscopic Implications of Spinâ€“Orbit Coupling Effects. Journal of Chemical Theory and Computation, 2018, 14, 1510-1522. | 2.3 | 8 |
| 5 | A four-component Fock-space coupled cluster investigation of the XMn(CO)5, (X = Cl, Br and I) photoelectron spectra. Chemical Physics, 2017, 482, 339-345. | 0.9 | 0 |
| 6 | Relativistic decay widths of autoionization processes: The relativistic FanoADC-Stieltjes method. Journal of Chemical Physics, 2015, 142, 144106. | 1.2 | 13 |
| 7 | Calculation of the lowest electronic excitations of the alkaline earth metals using the relativistic polarization propagator. Chemical Physics, 2015, 455, 7-16. | 0.9 | 1 |
| 8 | A four-component Fock-space coupled cluster investigation of the HM(CO)<sub>5</sub>, (M = Mn, Re) photoelectron spectra. Molecular Physics, 2015, 113, 3431-3437. | 0.8 | 4 |
| 9 | Plasmons in molecules: Microscopic characterization based on orbital transitions and momentum conservation. Journal of Chemical Physics, 2014, 141, 104101. | 1.2 | 26 |
| 10 | Communication: Electron transfer mediated decay enabled by spin-orbit interaction in small krypton/xenon clusters. Journal of Chemical Physics, 2014, 140, 161103. | 1.2 | 4 |
| 11 | The relativistic polarization propagator for the calculation of electronic excitations in heavy systems. Journal of Chemical Physics, 2014, 140, 084108. | 1.2 | 13 |
| 12 | A Theoretical DFTâ€Based and Experimental Study of the Transmetalation Step in Au/Pdâ€Mediated Crossâ€Coupling Reactions. Chemistry - A European Journal, 2013, 19, 15290-15303. | 1.7 | 49 |
| 13 | Ultrafast branching in the excited state of coumarin and umbelliferone. Physical Chemistry Chemical Physics, 2013, 15, 17846. | 1.3 | 48 |
| 14 | Interatomic decay of inner-valence ionized states in ArXe clusters: Relativistic approach. Journal of Chemical Physics, 2013, 138, 014305. | 1.2 | 15 |
| 15 | Electronic structure and UV spectrum of hexachloroplatinate dianions in vacuo. Journal of Chemical Physics, 2013, 139, 194310. | 1.2 | 12 |
| 16 | Strong configuration interaction in the double ionization spectra of noble gases studied by the relativistic propagator method. Physical Review A, 2012, 85, . | 1.0 | 9 |
| 17 | Spinâ€“orbit effects, electronic decay and breakdown phenomena in the photoelectron spectra of iodomethane. Chemical Physics, 2012, 407, 39-45. | 0.9 | 10 |
| 18 | Theoretical insights into the superior activity of gold catalysts and reactions of organogold intermediates with electrophiles. Faraday Discussions, 2011, 152, 179. | 1.6 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Gold Catalysis: Hydrolysis of Di(alkoxy)carbenium Ion Intermediates as a Sensor for the Electronic Properties of Gold(I) Complexes. Organometallics, 2011, 30, 5894-5903. | 1.1 | 78 |
| 20 | A New Insight into Gold(I)â€Catalyzed Hydration of Alkynes: Proton Transfer. ChemCatChem, 2010, 2, 1226-1230. | 1.8 | 186 |
| 21 | Nonadditivity and anisotropy of the polarizability of clusters: Relativistic finite-field calculations for the Xe dimer. Physical Review A, 2010, 81, . | 1.0 | 5 |
| 22 | Possible electronic decay channels in the ionization spectra of small clusters composed of Ar and Xe: A four-component relativistic treatment. Journal of Chemical Physics, 2010, 133, 014303. | 1.2 | 13 |
| 23 | The four-component two-particle propagator for the calculation of double-ionization spectra of heavy-element compounds: I. Method. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 205102. | 0.6 | 16 |
| 24 | Jahnâ€“Teller distortions in the photodetachment spectrum of PtCl62â^': A four-component relativistic study. Journal of Chemical Physics, 2009, 131, 044322. | 1.2 | 6 |
| 25 | Fully Relativistic, Comparative Investigation of Gold and Platinum Alkyne Complexes of Relevance for the Catalysis of Nucleophilic Additions to Alkynes. Journal of Chemical Theory and Computation, 2009, 5, 2717-2725. | 2.3 | 192 |
| 26 | Photodetachment spectra of the PtX42â^'â€ˆ(X=F,Cl,Br) dianions and their Jahnâ€“Teller distortions: A fully relativistic study. Journal of Chemical Physics, 2008, 129, 174302. | 1.2 | 11 |
| 27 | Possible electronic decay channels in the ionization spectra of small clusters composed of Ar and Kr: A four-component relativistic treatment. Journal of Chemical Physics, 2008, 129, 024304. | 1.2 | 19 |
| 28 | PtF62â^' dianion and its detachment spectrum: A fully relativistic study. Journal of Chemical Physics, 2007, 126, 144310. | 1.2 | 11 |
| 29 | A fully relativistic study of the and photodetachment spectra. Chemical Physics, 2007, 338, 44-52. | 0.9 | 12 |
| 30 | Relativistic calculation of the SeH2 and TeH2 photoelectron spectra. Chemical Physics, 2006, 329, 256-265. | 0.9 | 5 |
| 31 | Ionization spectra and electronic decay in small iodide clusters: Fully relativistic results. Journal of Chemical Physics, 2006, 125, 034309. | 1.2 | 11 |
| 32 | The influence of relativistic effects on the ionization spectra of the alkali iodides. Chemical Physics Letters, 2005, 410, 423-429. | 1.2 | 9 |
| 33 | Effect of relativity on the ionization spectra of the xenon fluorides XeFn (n=2, 4, 6). Journal of Chemical Physics, 2005, 122, 214302. | 1.2 | 12 |
| 34 | Remarkable interplay of electron correlation and relativity in the photodetachment spectrum of PtCl62â^'. Journal of Chemical Physics, 2005, 122, 064311. | 1.2 | 16 |
| 35 | Calculation of Nuclear Quadrupole Coupling Constants. , 2004, , 279-291. | | 38 |
| 36 | Parallelization of four-component calculations. II. Symmetry-driven parallelization of the 4-Spinor CCSD algorithm. Journal of Computational Chemistry, 2003, 24, 754-759. | 1.5 | 19 |

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|---|---|---|---|
| 37 | Nuclear quadrupole moments for 27Al and 69Ga derived from four-component molecular coupled cluster calculations. Journal of Chemical Physics, 2001, 114, 10389-10395. | 1.2 | 39 |