# Tim Clark

## List of Publications by Citations



| | | | |
|---|---|---|---|
| 431 papers | 23,277 citations | 61 h-index | 141 g-index |
| 469 ext. papers | 25,450 ext. citations | 6.2 avg, IF | 7.19 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 431 | Efficient diffuse function-augmented basis sets for anion calculations. III. The 3-21+G basis set for first-row elements, Li–F. *Journal of Computational Chemistry*, **1983**, 4, 294-301 | 3.5 | 5477 |
| 430 | Halogen bonding: the sigma-hole. Proceedings of "Modeling interactions in biomolecules II", Prague, September 5th-9th, 2005. *Journal of Molecular Modeling*, **2007**, 13, 291-6 | 2 | 1726 |
| 429 | Halogen bonding: an electrostatically-driven highly directional noncovalent interaction. *Physical Chemistry Chemical Physics*, **2010**, 12, 7748-57 | 3.6 | 1239 |
| 428 | Halogen bonding and other σ-hole interactions: a perspective. *Physical Chemistry Chemical Physics*, **2013**, 15, 11178-89 | 3.6 | 1186 |
| 427 | σ-holes, π-holes and electrostatically-driven interactions. *Journal of Molecular Modeling*, **2012**, 18, 541-8 | 2 | 460 |
| 426 | Sigma-hole bonding: molecules containing group VI atoms. *Journal of Molecular Modeling*, **2007**, 13, 1033-8 | 2 | 421 |
| 425 | Molecular docking sites designed for the generation of highly crystalline covalent organic frameworks. *Nature Chemistry*, **2016**, 8, 310-316 | 17.6 | 338 |
| 424 | Carbon nanodots: toward a comprehensive understanding of their photoluminescence. *Journal of the American Chemical Society*, **2014**, 136, 17308-16 | 16.4 | 282 |
| 423 | Stabilization of methyl anions by first-row substituents. The superiority of diffuse function-augmented basis sets for anion calculations. *Journal of Computational Chemistry*, **1982**, 3, 363-371 | 3.5 | 241 |
| 422 | The σ-hole revisited. *Physical Chemistry Chemical Physics*, **2017**, 19, 32166-32178 | 3.6 | 222 |
| 421 | Directional Weak Intermolecular Interactions: σ-Hole Bonding. *Australian Journal of Chemistry*, **2010**, 63, 1598 | 1.2 | 222 |
| 420 | σ-Holes. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 13-20 | 7.9 | 219 |
| 419 | Mathematical modeling and physical reality in noncovalent interactions. *Journal of Molecular Modeling*, **2015**, 21, 52 | 2 | 199 |
| 418 | Odd-electron .sigma. bonds. *Journal of the American Chemical Society*, **1988**, 110, 1672-1678 | 16.4 | 183 |
| 417 | On the Enhanced Stability of the Guanine–Cytosine Base-Pair Radical Cation. *Journal of the American Chemical Society*, **1996**, 118, 7574-7577 | 16.4 | 178 |
| 416 | Hydration and Water Exchange of Zinc(II) Ions. Application of Density Functional Theory. *Journal of the American Chemical Society*, **1997**, 119, 7843-7850 | 16.4 | 158 |
| 415 | Principle and mechanism of direct porphyrin metalation: joint experimental and theoretical investigation. *Journal of the American Chemical Society*, **2007**, 129, 9476-83 | 16.4 | 156 |

| | | | |
|---|---|---|---|
| 414 | A numerical self-consistent reaction field (SCRF) model for ground and excited states in NDDO-based methods. *Journal of the American Chemical Society*, **1993**, 115, 9174-9181 | 16.4 | 154 |
| 413 | Unified model for singlet fission within a non-conjugated covalent pentacene dimer. *Nature Communications*, **2017**, 8, 15171 | 17.4 | 143 |
| 412 | An evaluation of the performance of diffuse function-augmented basis sets for second row elements, Na-Cl. *Journal of Computational Chemistry*, **1987**, 8, 1109-1116 | 3.5 | 137 |
| 411 | Why are dimethyl sulfoxide and dimethyl sulfone such good solvents?. *Journal of Molecular Modeling*, **2008**, 14, 689-97 | 2 | 136 |
| 410 | Synchronized Offset Stacking: A Concept for Growing Large-Domain and Highly Crystalline 2D Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2016**, 138, 16703-16710 | 16.4 | 135 |
| 409 | Opening and Closure of the Fullerene Cage in cis-Bisimino Adducts of C60: The Influence of the Addition Pattern and the Addend. *Chemistry - A European Journal*, **1996**, 2, 935-943 | 4.8 | 119 |
| 408 | Hole bonding: a physical interpretation. *Topics in Current Chemistry*, **2015**, 358, 19-42 | | 117 |
| 407 | Stabilization of Atomic Nitrogen Inside C60. *Angewandte Chemie International Edition in English*, **1997**, 36, 2835-2838 | | 115 |
| 406 | Polarization-induced holes and hydrogen bonding. *Journal of Molecular Modeling*, **2012**, 18, 2461-9 | 2 | 112 |
| 405 | Triazole bridges as versatile linkers in electron donor-acceptor conjugates. *Journal of the American Chemical Society*, **2011**, 133, 13036-54 | 16.4 | 103 |
| 404 | Solvatochromic covalent organic frameworks. *Nature Communications*, **2018**, 9, 3802 | 17.4 | 100 |
| 403 | Descriptors, physical properties, and drug-likeness. *Journal of Medicinal Chemistry*, **2002**, 45, 3345-55 | 8.3 | 98 |
| 402 | A perspective on quantum mechanics and chemical concepts in describing noncovalent interactions. *Physical Chemistry Chemical Physics*, **2018**, 20, 30076-30082 | 3.6 | 96 |
| 401 | Directional Charge-Carrier Transport in Oriented Benzodithiophene Covalent Organic Framework Thin Films. *ACS Nano*, **2017**, 11, 2706-2713 | 16.7 | 90 |
| 400 | Correct electrostatic treatment of noncovalent interactions: the importance of polarization. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 169-177 | 7.9 | 87 |
| 399 | Phosphonate- and carboxylate-based self-assembled monolayers for organic devices: a theoretical study of surface binding on aluminum oxide with experimental support. *ACS Applied Materials & Interfaces*, **2013**, 5, 6073-80 | 9.5 | 85 |
| 398 | Allyllithium, allylsodium, and allylmagnesium hydride: geometries and bonding. A comparative ab initio study. *Organometallics*, **1983**, 2, 1344-1351 | 3.8 | 83 |
| 397 | Molecular wires--impact of conjugation and implementation of molecular bottlenecks. *Chemical Society Reviews*, **2015**, 44, 988-98 | 58.5 | 78 |

| | | | |
|---|---|---|---|
| 396 | An Efficient Metadynamics-Based Protocol To Model the Binding Affinity and the Transition State Ensemble of G-Protein-Coupled Receptor Ligands. *Journal of Chemical Information and Modeling*, **2017**, 57, 1210-1217 | 6.1 | 77 |
| 395 | Conformational Control of Photoinduced Charge Separation within Phenothiazine–Pyrene Dyads. *Journal of Physical Chemistry A*, **2002**, 106, 7958-7970 | 2.8 | 77 |
| 394 | Halogen bonds and holes. *Faraday Discussions*, **2017**, 203, 9-27 | 3.6 | 76 |
| 393 | Prediction of the n-Octanol/Water Partition Coefficient, logP, Using a Combination of Semiempirical MO-Calculations and a Neural Network. *Journal of Molecular Modeling*, **1997**, 3, 142-155 | 2 | 76 |
| 392 | Local molecular properties and their use in predicting reactivity. *Journal of Molecular Modeling*, **2003**, 9, 342-7 | 2 | 76 |
| 391 | QM/NN QSPR models with error estimation: vapor pressure and logP. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1046-51 | | 76 |
| 390 | Switching on and off Interlayer Correlations and Porosity in 2D Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2019**, 141, 12570-12581 | 16.4 | 75 |
| 389 | The relationship between threshold voltage and dipolar character of self-assembled monolayers in organic thin-film transistors. *Journal of the American Chemical Society*, **2012**, 134, 12648-52 | 16.4 | 75 |
| 388 | Tuning electron transfer through p-phenyleneethynylene molecular wires. *Chemical Communications*, **2006**, 3202-4 | 5.8 | 75 |
| 387 | Evidence for Charge-Transfer Mediation in the Primary Events of Singlet Fission in a Weakly Coupled Pentacene Dimer. *CheM*, **2018**, 4, 1092-1111 | 16.2 | 74 |
| 386 | Evidence for an enol mechanism in a highly enantioselective Mannich-type reaction catalyzed by primary amine-thiourea. *Angewandte Chemie - International Edition*, **2008**, 47, 6624-8 | 16.4 | 72 |
| 385 | Enforcing Extended Porphyrin J-Aggregate Stacking in Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2018**, 140, 16544-16552 | 16.4 | 72 |
| 384 | Ab initio structures of allyllithium. *Journal of Organometallic Chemistry*, **1978**, 150, 1-6 | 2.3 | 70 |
| 383 | p-Phenyleneethynylene molecular wires: influence of structure on photoinduced electron-transfer properties. *Chemistry - A European Journal*, **2008**, 14, 6379-90 | 4.8 | 69 |
| 382 | Regression formulae for ab initio and density functional calculated chemical shifts. *Journal of Molecular Modeling*, **2005**, 11, 175-85 | 2 | 67 |
| 381 | Carbon Nanodots: Supramolecular Electron Donor-Acceptor Hybrids Featuring Perylenediimides. *Angewandte Chemie - International Edition*, **2015**, 54, 8292-7 | 16.4 | 66 |
| 380 | [2,2']paracyclophane-based conjugated molecular wires reveal molecular-junction behavior. *Journal of the American Chemical Society*, **2011**, 133, 2370-3 | 16.4 | 66 |
| 379 | Structure-guided development of heterodimer-selective GPCR ligands. *Nature Communications*, **2016**, 7, 12298 | 17.4 | 65 |

| | | | |
|---|---|---|---|
| 378 | Directional Noncovalent Interactions: Repulsion and Dispersion. *Journal of Chemical Theory and Computation*, **2013**, 9, 2264-75 | 6.4 | 64 |
| 377 | AM1* parameters for phosphorus, sulfur and chlorine. *Journal of Molecular Modeling*, **2003**, 9, 408-14 | 2 | 64 |
| 376 | Assessment of Popular DFT and Semiempirical Molecular Orbital Techniques for Calculating Relative Transition State Energies and Kinetic Product Distributions in Enantioselective Organocatalytic Reactions. *Journal of Chemical Theory and Computation*, **2011**, 7, 3586-95 | 6.4 | 63 |
| 375 | Improving the charge transport in self-assembled monolayer field-effect transistors: from theory to devices. *Journal of the American Chemical Society*, **2013**, 135, 4893-900 | 16.4 | 61 |
| 374 | A molecular placeholder strategy to access a family of transition-metal-functionalized vanadium oxide clusters. *Chemistry - A European Journal*, **2014**, 20, 12269-73 | 4.8 | 61 |
| 373 | Towards a next generation neglect of diatomic differential overlap based semiempirical molecular orbital technique. *Theoretical Chemistry Accounts*, **2003**, 110, 254-266 | 1.9 | 61 |
| 372 | Quo Vadis semiempirical MO-theory?. *Computational and Theoretical Chemistry*, **2000**, 530, 1-10 | | 61 |
| 371 | NDDO-Based CI Methods for the Prediction of Electronic Spectra and Sum-Over-States Molecular Hyperpolarization. *Israel Journal of Chemistry*, **1993**, 33, 435-448 | 3.4 | 61 |
| 370 | Blending through-space and through-bond coupling in [2,2']-paracyclophane-oligophenylenevinylene molecular wires. *Journal of the American Chemical Society*, **2013**, 135, 10372-81 | 16.4 | 60 |
| 369 | CypScore: Quantitative prediction of reactivity toward cytochromes P450 based on semiempirical molecular orbital theory. *ChemMedChem*, **2009**, 4, 657-69 | 3.7 | 60 |
| 368 | Role of Polarization in Halogen Bonds. *Australian Journal of Chemistry*, **2014**, 67, 451 | 1.2 | 59 |
| 367 | A rhenium-cyclohexane complex with preferential binding of axial C-H bonds: a probe into the relative ability of C-H, C-D, and C-C bonds as hyperconjugative electron donors?. *Angewandte Chemie - International Edition*, **2006**, 45, 4486-90 | 16.4 | 57 |
| 366 | Enthalpies of formation from B3LYP calculations. *Journal of Computational Chemistry*, **2004**, 25, 725-33 | 3.5 | 57 |
| 365 | Semiconductor Type A Photocatalysis: Role of Substrate Adsorption and the Nature of Photoreactive Surface Sites in Zinc Sulfide Catalyzed C C Coupling Reactions. *Chemistry - A European Journal*, **1999**, 5, 208-217 | 4.8 | 57 |
| 364 | Multicenter point charge model for high-quality molecular electrostatic potentials from AM1 calculations. *Journal of Computational Chemistry*, **1993**, 14, 503-509 | 3.5 | 57 |
| 363 | On bond-critical points in QTAIM and weak interactions. *Journal of Molecular Modeling*, **2018**, 24, 142 | 2 | 56 |
| 362 | An improved generalized AMBER force field (GAFF) for urea. *Journal of Molecular Modeling*, **2010**, 16, 1427-40 | 2 | 54 |
| 361 | Phenothiazine Pyrene Dyads: Photoinduced Charge Separation and Structural Relaxation in the CT State. *Journal of Physical Chemistry A*, **2003**, 107, 9530-9541 | 2.8 | 54 |

| | | | |
|---|---|---|---|
| 360 | Carbon Nanodots for Charge-Transfer Processes. *Accounts of Chemical Research*, **2019**, 52, 955-963 | 24.3 | 53 |
| 359 | Self-association and electron transfer in donor-acceptor dyads connected by meta-substituted oligomers. *Journal of the American Chemical Society*, **2009**, 131, 12218-29 | 16.4 | 53 |
| 358 | Searching for stable, five-coordinate aquated Al(III) species. Water exchange mechanism and effect of pH. *Inorganic Chemistry*, **2007**, 46, 1112-22 | 5.1 | 53 |
| 357 | Cocrystallization with Acetylene. The 1 : 1 Complex with Benzene: Crystal Growth, X-Ray Diffraction and Molecular Simulations. *Helvetica Chimica Acta*, **2003**, 86, 1085-1100 | 2 | 52 |
| 356 | Water Exchange Reactions and Hydrolysis of Hydrated Titanium(III) Ions. A Density Functional Theory Study. *Journal of Physical Chemistry A*, **1999**, 103, 9899-9905 | 2.8 | 52 |
| 355 | The isomeric structures of SiH2LiF. *Journal of Organometallic Chemistry*, **1980**, 191, 347-353 | 2.3 | 51 |
| 354 | Regioselektive Metallierung von Aromaten, II. Zweitmetallierung von 1-Lithionaphthalin und 9-Lithioanthracen. *Chemische Berichte*, **1983**, 116, 3283-3292 | | 50 |
| 353 | Electron transfer within 2,7-dinitronaphthalene radical anion. *Journal of the American Chemical Society*, **2004**, 126, 15431-8 | 16.4 | 49 |
| 352 | The activation of tertiary carboxamides in metal complexes: an experimental and theoretical study on the methanolysis of acylated bispicolylamine copper(II) complexes. *Inorganic Chemistry*, **2004**, 43, 4663-73 | 5.1 | 49 |
| 351 | A composite model for HERG blockade. *ChemMedChem*, **2008**, 3, 254-65 | 3.7 | 48 |
| 350 | A theoretical evaluation of the synergetic capto-dative stabilisation of free radicals. *Tetrahedron Letters*, **1980**, 21, 3681-3684 | 2 | 48 |
| 349 | The Electronic Structure of Amorphous Carbon Nanodots. *Journal of Physical Chemistry B*, **2015**, 119, 7258-65 | 3.4 | 47 |
| 348 | Simulating FRET from tryptophan: is the rotamer model correct?. *Journal of the American Chemical Society*, **2006**, 128, 5142-52 | 16.4 | 47 |
| 347 | Radical addition to alkene–metal cation complexes. *Journal of the Chemical Society Chemical Communications*, **1986**, 1774-1776 | | 47 |
| 346 | o-Iodoxybenzoic acid (IBX): pKa and proton-affinity analysis. *Angewandte Chemie - International Edition*, **2006**, 45, 2929-34 | 16.4 | 45 |
| 345 | Tuning the reorganization energy of electron transfer in supramolecular ensembles--metalloporphyrin, oligophenylenevinylenes, and fullerene--and the impact on electron transfer kinetics. *Nanoscale*, **2015**, 7, 2597-608 | 7.7 | 44 |
| 344 | Varying the Interpentacene Electronic Coupling to Tune Singlet Fission. *Journal of the American Chemical Society*, **2019**, 141, 6191-6203 | 16.4 | 42 |
| 343 | Amphiphilic perylene-calix[4]arene hybrids: synthesis and tunable self-assembly. *Journal of the American Chemical Society*, **2015**, 137, 3308-17 | 16.4 | 42 |

| | | | |
|---|---|---|---|
| 342 | EMPIRE: a highly parallel semiempirical molecular orbital program: 1: self-consistent field calculations. *Journal of Molecular Modeling*, **2014**, 20, 2331 | 2 | 42 |
| 341 | The morphology of integrated self-assembled monolayers and their impact on devices A computational and experimental approach. *Organic Electronics*, **2010**, 11, 1476-1482 | 3.5 | 42 |
| 340 | The carbenoid, CCl3Li, eschews tetrahedral structures. *Journal of the American Chemical Society*, **1979**, 101, 7747-7748 | 16.4 | 41 |
| 339 | Davydov splitting and singlet fission in excitonically coupled pentacene dimers. *Chemical Science*, **2019**, 10, 3854-3863 | 9.4 | 40 |
| 338 | Using carbon nanodots as inexpensive and environmentally friendly sensitizers in mesoscopic solar cells. *Nanoscale Horizons*, **2016**, 1, 220-226 | 10.8 | 40 |
| 337 | The coulombic hole model describes bonding in CXIY complexes completely. *Physical Chemistry Chemical Physics*, **2018**, 20, 22849-22855 | 3.6 | 40 |
| 336 | 2D-dynamic representation of DNA sequences. *Chemical Physics Letters*, **2007**, 442, 140-144 | 2.5 | 40 |
| 335 | Conformations and Tautomers of Tetracycline. *Journal of Physical Chemistry B*, **2003**, 107, 13743-13749 | 3.4 | 40 |
| 334 | N-methyl-B-mesityldibenzo-1,4-azaborinine: the first experimental structure of a 1,4-azaborinine derivative. *Journal of the Chemical Society Chemical Communications*, **1992**, 1247 | | 40 |
| 333 | Three electron bonds. I. The H2SSH radical cation. *Journal of Computational Chemistry*, **1981**, 2, 261-265 | 3.5 | 40 |
| 332 | Trifluoromethyl: An Amphiphilic Noncovalent Bonding Partner. *ChemPhysChem*, **2017**, 18, 772-784 | 3.2 | 39 |
| 331 | Template-dependent photochemical reactivity of molecular metal oxides. *Chemistry - A European Journal*, **2015**, 21, 8716-9 | 4.8 | 39 |
| 330 | Quantum-dot-sensitized solar cells: understanding linker molecules through theory and experiment. *Langmuir*, **2013**, 29, 2434-8 | 4 | 39 |
| 329 | Modern Molecular Mechanics and ab Initio Calculations on Benzylic and Cyclic Delocalized Cations. *Journal of Physical Chemistry A*, **1998**, 102, 8953-8963 | 2.8 | 39 |
| 328 | Fullerene van der Waals oligomers as electron traps. *Journal of the American Chemical Society*, **2014** , 136, 10890-3 | 16.4 | 38 |
| 327 | New molecular descriptors based on local properties at the molecular surface and a boiling-point model derived from them. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 658-68 | | 38 |
| 326 | The structure and stability of Si60 and Ge60 cages: a computational study. *Journal of Computational Chemistry*, **2003**, 24, 948-53 | 3.5 | 38 |
| 325 | Nature of the interaction of paramagnetic atoms (A=4N,4P,3O,3S) with systems and C60: A theoretical investigation of A???C6H6 and endohedral fullerenes A@C60. *Journal of Chemical Physics*, **2002**, 116, 10684-10691 | 3.9 | 38 |

| | | | |
|---|---|---|---|
| 324 | Y vs. cyclic delocalization in small ring dications and dianions: The dominance of charge repulsion over Huckel aromaticity. *Tetrahedron Letters*, **1982**, 23, 3547-3550 | 2 | 38 |
| 323 | Solvation largely accounts for the effect of N-alkylation on the properties of nickel(II/I) and chromium(III/II) cyclam complexes. *Inorganic Chemistry*, **2002**, 41, 2927-35 | 5.1 | 37 |
| 322 | A quantum mechanical/neural net model for boiling points with error estimation. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 457-62 | | 37 |
| 321 | A carbon-carbon hybrid - immobilizing carbon nanodots onto carbon nanotubes. *Chemical Science*, **2015**, 6, 6878-6885 | 9.4 | 36 |
| 320 | MO-Studies of enzyme reaction mechanisms. I. Model molecular orbital study of the cleavage of peptides by carboxypeptidase A. *Journal of Computational Chemistry*, **1992**, 13, 704-717 | 3.5 | 36 |
| 319 | Synthesis and evaluation of new guanidine-thiourea organocatalyst for the nitro-Michael reaction: Theoretical studies on mechanism and enantioselectivity. *Beilstein Journal of Organic Chemistry*, **2012**, 8, 1485-98 | 2.5 | 35 |
| 318 | Distribution moments of 2D-graphs as descriptors of DNA sequences. *Chemical Physics Letters*, **2007**, 443, 408-413 | 2.5 | 35 |
| 317 | AM1* parameters for aluminum, silicon, titanium and zirconium. *Journal of Molecular Modeling*, **2005**, 11, 439-56 | 2 | 35 |
| 316 | The Hole Coulombic Interpretation of Trihalide Anion Formation. *ChemPhysChem*, **2018**, 19, 3044-3049 | 3.2 | 35 |
| 315 | Multiple Binding Sites Contribute to the Mechanism of Mixed Agonistic and Positive Allosteric Modulators of the Cannabinoid CB1 Receptor. *Angewandte Chemie - International Edition*, **2018**, 57, 2580-2585 | 16.4 | 34 |
| 314 | VESPA: A new, fast approach to electrostatic potential-derived atomic charges from semiempirical methods. *Journal of Computational Chemistry*, **1997**, 18, 744-756 | 3.5 | 34 |
| 313 | Investigation of the Uncatalyzed Hydration of CO2 and First Approximations to the Active Site of Carbonic Anhydrase - A Combined Ab initio and DFT Study -. *Journal of Molecular Modeling*, **1996**, 2, 358-361 | 2 | 34 |
| 312 | Homology model adjustment and ligand screening with a pseudoreceptor of the human histamine H4 receptor. *ChemMedChem*, **2009**, 4, 820-7 | 3.7 | 33 |
| 311 | Evidence for an Enol Mechanism in a Highly Enantioselective Mannich-Type Reaction Catalyzed by Primary Amine Thiourea. *Angewandte Chemie*, **2008**, 120, 6726-6730 | 3.6 | 33 |
| 310 | Active-state models of ternary GPCR complexes: determinants of selective receptor-G-protein coupling. *PLoS ONE*, **2013**, 8, e67244 | 3.7 | 33 |
| 309 | Does metal ion complexation make radical clocks run fast?. *Journal of the American Chemical Society* , **2003**, 125, 2809-16 | 16.4 | 32 |
| 308 | Quantum mechanical/molecular mechanical (QM/MM) docking: an evaluation for known test systems. *Molecular Physics*, **2003**, 101, 2469-2480 | 1.7 | 32 |
| 307 | A temperature-dependent quantum mechanical/neural net model for vapor pressure. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1053-9 | | 32 |

| | | | |
|---|---|---|---|
| 306 | Double lithium bridging: The structure of 1,4-dilithio-1,4-diphenyl-cis-2-butene. *Journal of Organometallic Chemistry*, **1985**, 280, C6-C10 | 2.3 | 32 |
| 305 | A Three-Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. *Angewandte Chemie - International Edition*, **2016**, 55, 8008-12 | 16.4 | 32 |
| 304 | The local electron affinity for non-minimal basis sets. *Journal of Molecular Modeling*, **2010**, 16, 1231-8 | 2 | 31 |
| 303 | Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods. *International Journal of Quantum Chemistry*, **1999**, 75, 17-31 | 2.1 | 31 |
| 302 | The natural atomic orbital point charge model for PM3: Multipole moments and molecular electrostatic potentials. *Journal of Computational Chemistry*, **1994**, 15, 1064-1073 | 3.5 | 31 |
| 301 | The solvent effect on the electronic nature of 1,3-dipoles: an ab initio SCRF study. *Journal of the American Chemical Society*, **1989**, 111, 9107-9109 | 16.4 | 31 |
| 300 | Polarization, donor-acceptor interactions, and covalent contributions in weak interactions: a clarification. *Journal of Molecular Modeling*, **2017**, 23, 297 | 2 | 30 |
| 299 | The Important Role of Active Site Water in the Catalytic Mechanism of Human Carbonic Anhydrase II □A Semiempirical MO Approach to the Hydration of CO2 □ *Journal of Molecular Modeling*, **1998**, 4, 355-365 | 2 | 30 |
| 298 | AM1* parameters for copper and zinc. *Journal of Molecular Modeling*, **2007**, 13, 965-79 | 2 | 30 |
| 297 | In silico prediction of buffer solubility based on quantum-mechanical and HQSAR- and topology-based descriptors. *Journal of Chemical Information and Modeling*, **2006**, 46, 648-58 | 6.1 | 30 |
| 296 | QSAR and QSPR based solely on surface properties?. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 519-25 | 2.8 | 30 |
| 295 | NO binding to cobalamin: influence of the metal oxidation state. *Inorganic Chemistry*, **2004**, 43, 2828-33 | 5.1 | 30 |
| 294 | Indentation and self-healing mechanisms of a self-assembled monolayer--a combined experimental and modeling study. *Journal of the American Chemical Society*, **2014**, 136, 10718-27 | 16.4 | 29 |
| 293 | Molecular dynamics simulations of the effect of the G-protein and diffusible ligands on the □-adrenergic receptor. *Journal of Molecular Biology*, **2011**, 414, 611-23 | 6.5 | 29 |
| 292 | Control over charge transfer through molecular wires by temperature and chemical structure modifications. *ACS Nano*, **2010**, 4, 6449-62 | 16.7 | 29 |
| 291 | Mediating Reductive Charge Shift Reactions in Electron Transport Chains. *Journal of the American Chemical Society*, **2017**, 139, 17474-17483 | 16.4 | 28 |
| 290 | Carboxylate Ion Pairing with Alkali-Metal Ions for □Lactoglobulin and Its Role on Aggregation and Interfacial Adsorption. *Journal of Physical Chemistry B*, **2015**, 119, 5505-17 | 3.4 | 28 |
| 289 | Doped polycyclic aromatic hydrocarbons as building blocks for nanoelectronics: a theoretical study. *Journal of Organic Chemistry*, **2013**, 78, 1894-902 | 4.2 | 28 |

| | | | |
|---|---|---|---|
| 288 | 3D-QSAR based on quantum-chemical molecular fields: toward an improved description of halogen interactions. *Journal of Chemical Information and Modeling*, **2012**, 52, 2441-53 | 6.1 | 28 |
| 287 | Additive NDDO-based atomic polarizability model. *International Journal of Quantum Chemistry*, **2000**, 77, 473-497 | 2.1 | 28 |
| 286 | Geometries and Energies of Dilithioethylene Isomers and of Vinyl Lithium. An Ab Initio Study. *Israel Journal of Chemistry*, **1980**, 20, 43-50 | 3.4 | 28 |
| 285 | Vinyl spacers tuning electron transfer through fluorene-based molecular wires. *Energy and Environmental Science*, **2011**, 4, 765 | 35.4 | 27 |
| 284 | Dispersion treatment for NDDO-based semiempirical MO techniques. *International Journal of Quantum Chemistry*, **2006**, 106, 1208-1216 | 2.1 | 27 |
| 283 | Active-state model of a dopamine D2 receptor-G protein complex stabilized by aripiprazole-type partial agonists. *PLoS ONE*, **2014**, 9, e100069 | 3.7 | 26 |
| 282 | Semiempirical UNO-CAS and UNO-CI: method and applications in nanoelectronics. *Journal of Physical Chemistry A*, **2011**, 115, 11303-12 | 2.8 | 26 |
| 281 | Stabilisierung von atomarem Stickstoff im Innenraum von C60. *Angewandte Chemie*, **1997**, 109, 2858-2861 | 3.6 | 26 |
| 280 | Molecular orbital studies of enzyme mechanisms. II. Catalytic oxidation of alcohols by liver alcohol dehydrogenase. *Journal of Computational Chemistry*, **1993**, 14, 392-400 | 3.5 | 26 |
| 279 | Condensed-phase radical anions. *Faraday Discussions of the Chemical Society*, **1984**, 78, 203 | | 26 |
| 278 | The structures of the carbenoid CH2FLi: ab initio MO calculations. *Journal of the Chemical Society Chemical Communications*, **1979**, 883 | | 26 |
| 277 | Highly Regioselective Alkylation of Hexabenzocoronenes: Fundamental Insights into the Covalent Chemistry of Graphene. *Angewandte Chemie - International Edition*, **2017**, 56, 12184-12190 | 16.4 | 25 |
| 276 | Analysis of diatomic bond dissociation and formation in terms of the reaction force and the position-dependent reaction force constant. *Journal of Molecular Modeling*, **2009**, 15, 701-6 | 2 | 25 |
| 275 | A QSPR-approach to the estimation of the pK(HB) of six-membered nitrogen-heterocycles using quantum mechanically derived descriptors. *Journal of Molecular Modeling*, **2002**, 8, 95-101 | 2 | 25 |
| 274 | P(6) Manganocene and P(3) Cymantrene: Consequences of the Inclusion of Phosphorus Atoms in Mn-Coordinated Cyclopentadienyl Ligands This work was supported by the Deutsche Forschungsgemeinschaft and the Fonds der Chemischen Industrie. A.E., M.H., and M.Z. thank the DFG-Graduiertenkolleg ("Phosphorchemie als Bindeglied verschiedener chemischer Disziplinen" of the University of Kaiserslautern) and M.Z. also thanks the Studienstiftung des Deutschen Volkes for fellowships. *Angewandte Chemie - International Edition*, **2000**, 39, 2087-2091 | 16.4 | 25 |
| 273 | -Aromaticity in Three-Membered Rings. *Journal of Molecular Modeling*, **2000**, 6, 133-149 | 2 | 25 |
| 272 | Conformational Analysis of Tetracycline using Molecular Mechanical and Semiempirical MO-Calculations. *Journal of Molecular Modeling*, **1999**, 5, 46-62 | 2 | 25 |
| 271 | Predicting the effects of basepair mutations in DNA-protein complexes by thermodynamic integration. *Biophysical Journal*, **2011**, 101, 1130-8 | 2.9 | 24 |

| | | | |
|---|---|---|---|
| 270 | Enhanced 3D-Databases: A Fully Electrostatic Database of AM1-Optimized Structures. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 1214-1217 | | 24 |
| 269 | Theoretical study of the carbenoid CH2FLi: Structures and energies of the stable configurations and transition states. *Chemical Physics Letters*, **1983**, 102, 148-154 | 2.5 | 24 |
| 268 | C4Li4, Tetralithiotetrahedran?. *Angewandte Chemie*, **1978**, 90, 306-307 | 3.6 | 24 |
| 267 | Pentacenes: A Molecular Ruler for Singlet Fission. *Trends in Chemistry*, **2019**, 1, 11-21 | 14.8 | 23 |
| 266 | Understanding and Controlling Short- and Long-Range Electron/Charge-Transfer Processes in Electron Donor-Acceptor Conjugates. *Journal of the American Chemical Society*, **2020**, 142, 7898-7911 | 16.4 | 23 |
| 265 | EMPIRE: a highly parallel semiempirical molecular orbital program: 2: periodic boundary conditions. *Journal of Molecular Modeling*, **2015**, 21, 144 | 2 | 23 |
| 264 | Mixed self-assembled monolayer of molecules with dipolar and acceptor character influence on hysteresis and threshold voltage in organic thin-film transistors. *Applied Physics Letters*, **2012**, 100, 063302 | 3.4 | 23 |
| 263 | An analytical, variable resolution, complete description of static molecules and their intermolecular binding properties. *Journal of Chemical Information and Modeling*, **2005**, 45, 1010-6 | 6.1 | 23 |
| 262 | Energy Efficient Ultrahigh Flux Separation of Oily Pollutants from Water with Superhydrophilic Nanoscale Metal-Organic Framework Architectures. *Angewandte Chemie - International Edition*, **2021**, 60, 5519-5526 | 16.4 | 23 |
| 261 | An unsymmetrical pentacene derivative with ambipolar behavior in organic thin-film transistors. *Chemical Communications*, **2013**, 49, 6725-7 | 5.8 | 22 |
| 260 | A stacked porphyrin-fullerene electron donor-acceptor conjugate that features a surprising frozen geometry. *Chemistry - A European Journal*, **2012**, 18, 14008-16 | 4.8 | 22 |
| 259 | Insolubility classification with accurate prediction probabilities using a MetaClassifier. *Journal of Chemical Information and Modeling*, **2010**, 50, 404-14 | 6.1 | 22 |
| 258 | Chemistry of Convex versus Concave Carbon: The Reactive Exterior and the Inert Interior of C60. *Journal of Molecular Modeling*, **1997**, 3, 415-422 | 2 | 22 |
| 257 | Aeromonas proteolytica aminopeptidase: an investigation of the mode of action using a quantum mechanical/molecular mechanical approach. *Biochemistry*, **2004**, 43, 5414-27 | 3.2 | 22 |
| 256 | Ground-state tautomerism and rotational isomerization in 4,5-dimethyl-2-(2-hydroxyphenyl)imidazole in the gas phase and in polar solvents: a theoretical study of the aromaticity, intramolecular hydrogen-bond strength and differential solute solvent interactions. *Physical Chemistry Chemical Physics*, **2001**, 3, 3569-3579 | 3.6 | 22 |
| 255 | Theoretical Study of the Water Exchange Reaction on Divalent Zinc Ion using Density Functional Theory. *Journal of Molecular Modeling*, **1996**, 2, 354-357 | 2 | 22 |
| 254 | On-off switch of charge-separated states of pyridine-vinylene-linked porphyrin-C conjugates detected by EPR. *Chemical Science*, **2015**, 6, 5994-6007 | 9.4 | 21 |
| 253 | Integrating metalloporphycenes into p-type NiO-based dye-sensitized solar cells. *Chemical Communications*, **2014**, 50, 11339-42 | 5.8 | 21 |

| | | | |
|---|---|---|---|
| 252 | Self-assembly of structurally persistent micelles is controlled by specific-ion effects and hydrophobic guests. *Langmuir*, **2010**, 26, 10460-6 | 4 | 21 |
| 251 | Ambiphilicity: a characteristic reactivity principle of pi-bound phosphorus heterocycles. *Angewandte Chemie - International Edition*, **2002**, 41, 4047-52 | 16.4 | 21 |
| 250 | The Reaction Mechanism of Bovine Lens Leucine Aminopeptidase. *Journal of Physical Chemistry B*, **2002**, 106, 8815-30 | 3.4 | 21 |
| 249 | The Mode of Action of Phospholipase A2: Semiempirical MO Calculations Including the Protein Environment. *Journal of Physical Chemistry B*, **2000**, 104, 1349-1361 | 3.4 | 21 |
| 248 | Strategies for improving responses to DNA vaccines. *Journal of Molecular Modeling*, **1999**, 5, 1-8 | 2 | 21 |
| 247 | Twisting in alkyl-substituted olefin cation radicals. *Journal of the American Chemical Society*, **1988**, 110, 868-870 | 16.4 | 21 |
| 246 | Three-Electron bonds. II. SS and SCL three-electron bonds. *Journal of Computational Chemistry*, **1982**, 3, 112-116 | 3.5 | 21 |
| 245 | Hydroboration; An ab initio study of the reaction of BH3 with ethylene. *Journal of Organometallic Chemistry*, **1978**, 156, 191-202 | 2.3 | 21 |
| 244 | Identification of the Beer Component Hordenine as Food-Derived Dopamine D2 Receptor Agonist by Virtual Screening a 3D Compound Database. *Scientific Reports*, **2017**, 7, 44201 | 4.9 | 20 |
| 243 | Radical Arylation of Anilines and Pyrroles via Aryldiazotates. *Chemistry - A European Journal*, **2017**, 23, 9647-9656 | 4.8 | 20 |
| 242 | Investigating allosteric effects on the functional dynamics of β2-adrenergic ternary complexes with enhanced-sampling simulations. *Chemical Science*, **2017**, 8, 4019-4026 | 9.4 | 20 |
| 241 | Precise control of intramolecular charge-transport: the interplay of distance and conformational effects. *Chemistry - A European Journal*, **2013**, 19, 7575-86 | 4.8 | 20 |
| 240 | Quantum mechanics-based properties for 3D-QSAR. *Journal of Chemical Information and Modeling*, **2013**, 53, 1486-502 | 6.1 | 20 |
| 239 | Silicon Lewis Acid Catalyzed [3+2] Cycloaddition Reactions of Hydrazones/Cyclopentadiene: Mild Access to Pyrazolidine Derivatives. *European Journal of Organic Chemistry*, **2011**, 2011, 3706-3709 | 3.2 | 20 |
| 238 | A consistent dataset of kinetic solubilities for early-phase drug discovery. *ChemMedChem*, **2009**, 4, 1529-36 | 3.7 | 20 |
| 237 | AM1* parameters for bromine and iodine. *Journal of Molecular Modeling*, **2009**, 15, 295-308 | 2 | 20 |
| 236 | Lithium cation as radical-polymerization catalyst. *Journal of the American Chemical Society*, **2006**, 128, 11278-85 | 16.4 | 20 |
| 235 | Reactions of polyanions derived from alkylbenzenes. *Journal of the American Chemical Society*, **1984**, 106, 361-367 | 16.4 | 20 |

| | | | |
|---|---|---|---|
| 234 | Identification of Two Distinct Sites for Antagonist and Biased Agonist Binding to the Human Chemokine Receptor CXCR3. *Angewandte Chemie - International Edition*, **2016**, 55, 15277-15281 | 16.4 | 19 |
| 233 | Why do cationic hydridoiridium(III) complexes with beta-aminophosphane ligands favour the transfer hydrogenation of ketones over the direct "H2-hydrogenation"?--A computational approach. *Chemistry - A European Journal*, **2008**, 14, 8898-903 | 4.8 | 19 |
| 232 | Rock around the Ring: An Experimental and Theoretical Study of the Molecular Dynamics of Stannyltriphospholes with Chiral Tin Substituents. *European Journal of Inorganic Chemistry*, **2008**, 2008, 2225-2237 | 2.3 | 19 |
| 231 | The formation of endo-complexes between calixarenes and amines--a reinvestigation. *Journal of Molecular Modeling*, **2006**, 12, 739-47 | 2 | 19 |
| 230 | Three-electron bonds. III. Phosphorus and chlorine  radical cations. *Journal of Computational Chemistry*, **1983**, 4, 404-409 | 3.5 | 19 |
| 229 | Proposal for the mechanism of inversion of alkyl-lithiums. *Journal of the Chemical Society Chemical Communications*, **1978**, 137 | | 19 |
| 228 | From benzodithiophene to diethoxy-benzodithiophene covalent organic frameworks structural investigations. *CrystEngComm*, **2016**, 18, 4295-4302 | 3.3 | 18 |
| 227 | Molecular dynamics simulations of liquid phase interfaces: understanding the structure of the glycerol/water-dodecane system. *Langmuir*, **2013**, 29, 11898-907 | 4 | 18 |
| 226 | MNDO-Like Semiempirical Molecular Orbital Theory and Its Application to Large Systems **2011**, 259-286 | | 18 |
| 225 | Counterions control the self-assembly of structurally persistent micelles: theoretical prediction and experimental observation of stabilization by sodium ions. *Chemistry - A European Journal*, **2009**, 15, 8586-92 | 4.8 | 18 |
| 224 | Sodium effect on self-organization of amphiphilic carboxylates: formation of structured micelles and superlattices. *Chemistry - A European Journal*, **2010**, 16, 9544-54 | 4.8 | 18 |
| 223 | Molecular orbital studies of electron-transfer reactions. *Journal of the Chemical Society, Faraday Transactions*, **1994**, 90, 1783 | | 18 |
| 222 | Catalysis of the ring-opening and isomerization of cyclopropane by complexation with metal radical cations: an ab initio study. *Journal of the American Chemical Society*, **1992**, 114, 10897-10902 | 16.4 | 18 |
| 221 | Measurement of the rotational barrier of a tetraalkylhydrazine radical cation. *Journal of the American Chemical Society*, **1983**, 105, 5928-5929 | 16.4 | 18 |
| 220 | Stabilization of methyl cations by second row substituents. *Tetrahedron Letters*, **1979**, 20, 4641-4644 | 2 | 18 |
| 219 | Structures of lithiomethanol and lithiomethylamine; and an ab initio study. *Journal of the Chemical Society Chemical Communications*, **1981**, 579-581 | | 18 |
| 218 | Multiply bonded metal(II) acetate (rhodium, ruthenium, and molybdenum) complexes with the trans-1,2-bis(N-methylimidazol-2-yl)ethylene ligand. *Inorganic Chemistry*, **2014**, 53, 12305-14 | 5.1 | 17 |
| 217 | Neighboring group stabilization by sigma-holes. *Journal of Molecular Modeling*, **2010**, 16, 559-65 | 2 | 17 |

| | | | |
|---|---|---|---|
| 216 | Empirical force field and ab initio calculations on allyl cations. *Journal of Computational Chemistry*, **1997**, 18, 533-551 | 3.5 | 17 |
| 215 | ParaFrag--an approach for surface-based similarity comparison of molecular fragments. *Journal of Molecular Modeling*, **2008**, 14, 547-58 | 2 | 17 |
| 214 | The Cyclooligomerisation of Acetylene at Metal Centres. *European Journal of Inorganic Chemistry*, **2008**, 2008, 2874-2883 | 2.3 | 17 |
| 213 | The Quadricyclane to Norbornadiene Radical Cation Rearrangement: an Ab Initio and Density Functional Study.. *Acta Chemica Scandinavica*, **1997**, 51, 646-652 | | 17 |
| 212 | Charge-Gating Dibenzothiophene-S,S-dioxide Bridges in Electron Donor□Bridge□Acceptor Conjugates. *Journal of Physical Chemistry C*, **2017**, 121, 13557-13569 | 3.8 | 16 |
| 211 | Thermochromic and solvatochromic properties of Lindqvist polyoxometalates. *Chemical Communications*, **2015**, 51, 13702-5 | 5.8 | 16 |
| 210 | 20D-dynamic representation of protein sequences. *Genomics*, **2016**, 107, 16-23 | 4.3 | 16 |
| 209 | Explicit Inclusion of Polarizing Electric Fields in □and □Hole Interactions. *Journal of Physical Chemistry A*, **2019**, 123, 10123-10130 | 2.8 | 16 |
| 208 | Effect of Structure and Disorder on the Charge Transport in Defined Self-Assembled Monolayers of Organic Semiconductors. *ACS Nano*, **2017**, 11, 8747-8757 | 16.7 | 16 |
| 207 | Formation of a protective layer during IEC(b) test of epoxy resin loaded with silica nanoparticles. *IEEE Transactions on Dielectrics and Electrical Insulation*, **2012**, 19, 786-792 | 2.3 | 16 |
| 206 | AM1 parameters for cobalt and nickel. *Journal of Molecular Modeling*, **2010**, 16, 29-47 | 2 | 16 |
| 205 | Similarity studies of DNA sequences using genetic methods. *Chemical Physics Letters*, **2007**, 445, 68-73 | 2.5 | 16 |
| 204 | Molecular dynamics simulation links conformation of a pore-flanking region to hyperekplexia-related dysfunction of the inhibitory glycine receptor. *Chemistry and Biology*, **2004**, 11, 1339-50 | | 16 |
| 203 | Multipole electrostatic model for MNDO-like techniques with minimal valence spd-basis sets. *Theoretical Chemistry Accounts*, **2005**, 114, 159-168 | 1.9 | 16 |
| 202 | Electrostatic catalysis of oxidation reactions by metal cations: an ab initio study. *Journal of the American Chemical Society*, **1991**, 113, 2422-2425 | 16.4 | 16 |
| 201 | A push-pull unsymmetrical subphthalocyanine dimer. *Chemical Science*, **2015**, 6, 5571-5577 | 9.4 | 15 |
| 200 | Theoretical and experimental insights into the surface chemistry of semiconductor quantum dots. *Langmuir*, **2013**, 29, 15450-6 | 4 | 15 |
| 199 | Dendronizing and metalating trans-2 C60 tetraaryl porphyrins--a versatile approach toward water-soluble donor-acceptor conjugates. *Chemistry - A European Journal*, **2010**, 16, 10797-807 | 4.8 | 15 |

| | | | |
|---|---|---|---|
| 198 | A Detailed Study of VESPA Electrostatic Potential-Derived Atomic Charges. *Journal of Molecular Modeling*, **1995**, 1, 176-187 | 2 | 15 |
| 197 | Semiempirical Molecular Orbital Theory: Facts, Myths and Legends **1993**, 369-380 | | 15 |
| 196 | Dihydroacepentalendiid, das Dianion des Acepentalens. *Angewandte Chemie*, **1986**, 98, 734-735 | 3.6 | 15 |
| 195 | Isomeric structures of the carbenoid, CHF2Li. *Tetrahedron Letters*, **1979**, 20, 4963-4966 | 2 | 15 |
| 194 | Singlet Fission in Pyrene-Fused Azaacene Dimers. *Angewandte Chemie - International Edition*, **2020**, 59, 1113-1117 | 16.4 | 15 |
| 193 | Accurate Intermolecular Potential for the C Dimer: The Performance of Different Levels of Quantum Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 274-285 | 6.4 | 14 |
| 192 | How To Make Nitroaromatic Compounds Glow: Next-Generation Large X-Shaped, Centrosymmetric Diketopyrrolopyrroles. *Angewandte Chemie - International Edition*, **2020**, 59, 16104-16113 | 16.4 | 14 |
| 191 | Chromophore Multiplication To Enable Exciton Delocalization and Triplet Diffusion Following Singlet Fission in Tetrameric Pentacene. *Angewandte Chemie - International Edition*, **2019**, 58, 15263-15267 | 16.4 | 14 |
| 190 | Economical and accurate protocol for calculating hydrogen-bond-acceptor strengths. *Journal of Chemical Information and Modeling*, **2013**, 53, 3262-72 | 6.1 | 14 |
| 189 | Modeling charge transport in C60-based self-assembled monolayers for applications in field-effect transistors. *Journal of Chemical Physics*, **2014**, 140, 204702 | 3.9 | 14 |
| 188 | A surface-integral model for log P OW. *Journal of Chemical Information and Modeling*, **2010**, 50, 429-36 | 6.1 | 14 |
| 187 | AM1* parameters for vanadium and chromium. *Journal of Molecular Modeling*, **2009**, 15, 1253-69 | 2 | 14 |
| 186 | o-Iodoxybenzoic Acid (IBX): pKa and Proton-Affinity Analysis. *Angewandte Chemie*, **2006**, 118, 2995-3000 | 3.6 | 14 |
| 185 | Nitrite impurities are responsible for the reaction observed between vitamin B12 and nitric oxide in acidic aqueous solution. *Inorganic Chemistry*, **2006**, 45, 7869-76 | 5.1 | 14 |
| 184 | Catalysis of closed-shell reactions by complexation with metal radical cations. *Journal of the American Chemical Society*, **1989**, 111, 761-763 | 16.4 | 14 |
| 183 | The nature of the counterion in butyllithium/potassium t-alkoxide reaction mixtures: An ESR study. *Journal of Organometallic Chemistry*, **1984**, 273, C1-C3 | 2.3 | 14 |
| 182 | (CH2LiF)2: the effect of dimerization on the structure and dissociation energy of carbenoids. *Journal of the Chemical Society Chemical Communications*, **1982**, 882-884 | | 14 |
| 181 | Solvent-Dependent Singlet Fission in Diketopyrrolopyrrole Dimers: A Mediating Charge Transfer versus a Trapping Symmetry-Breaking Charge Separation. *Advanced Energy Materials*, **2020**, 10, 2001496 | 21.8 | 14 |

| | | | |
|---|---|---|---|
| 180 | Strongly Directing Substituents in the Radical Arylation of Substituted Benzenes. *Journal of Organic Chemistry*, **2016**, 81, 9785-9791 | 4.2 | 14 |
| 179 | Differences between G-Protein-Stabilized Agonist-GPCR Complexes and their Nanobody-Stabilized Equivalents. *Angewandte Chemie - International Edition*, **2017**, 56, 9008-9012 | 16.4 | 13 |
| 178 | Odd-Electron Bonds. *ChemPhysChem*, **2017**, 18, 2766-2771 | 3.2 | 13 |
| 177 | A combined activation mechanism for the glucagon receptor. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 15414-15422 | 11.5 | 13 |
| 176 | Sharpening the toolbox of computational chemistry: a new approximation of critical f-values for multiple linear regression. *Journal of Chemical Information and Modeling*, **2009**, 49, 28-34 | 6.1 | 13 |
| 175 | An ab initio and density functional theory study of radical-clock reactions. *Journal of Organic Chemistry*, **2008**, 73, 1536-45 | 4.2 | 13 |
| 174 | Monitoring biological membrane-potential changes: a CI QM/MM study. *Journal of Physical Chemistry B*, **2008**, 112, 2445-55 | 3.4 | 13 |
| 173 | Surface-integral QSPR models: local energy properties. *Journal of Chemical Information and Modeling*, **2005**, 45, 1053-60 | 6.1 | 13 |
| 172 | Near-infrared Fourier transform surface-enhanced Raman scattering spectroscopy of 1,4-benzodiazepine drugs employing gold films over nanospheres. *Journal of Raman Spectroscopy*, **2004**, 35, 368-383 | 2.3 | 13 |
| 171 | SAM1 semiempirical calculations on the mechanism of cytochrome P450 metabolism. *Computational and Theoretical Chemistry*, **2001**, 541, 263-281 | | 13 |
| 170 | Cation-Mediated, Substituent-Controlled, C2□7 Cycloaromatization of an Enyne□Allene□ *Journal of Organic Chemistry*, **1999**, 64, 6166-6168 | 4.2 | 13 |
| 169 | Stabilization of methyl anions by first row substituents. *Tetrahedron Letters*, **1980**, 21, 743-746 | 2 | 13 |
| 168 | Influence of the heavy-atom effect on singlet fission: a study of platinum-bridged pentacene dimers. *Chemical Science*, **2019**, 10, 11130-11140 | 9.4 | 13 |
| 167 | Perylene-Monoimides: Singlet Fission Down-Conversion Competes with Up-Conversion by Geminate Triplet-Triplet Recombination. *Journal of Physical Chemistry A*, **2020**, 124, 5727-5736 | 2.8 | 12 |
| 166 | Tuning the Carbon Nanotube Selectivity: Optimizing Reduction Potentials and Distortion Angles in Perylenediimides. *Journal of the American Chemical Society*, **2018**, 140, 5427-5433 | 16.4 | 12 |
| 165 | Opposing Electronic and Nuclear Quantum Effects on Hydrogen Bonds in H O and D O. *ChemPhysChem*, **2019**, 20, 2461-2465 | 3.2 | 12 |
| 164 | Self-consistent field convergence for proteins: a comparison of full and localized-molecular-orbital schemes. *Journal of Molecular Modeling*, **2014**, 20, 2159 | 2 | 12 |
| 163 | G-Protein coupled receptors: answers from simulations. *Beilstein Journal of Organic Chemistry*, **2017**, 13, 1071-1078 | 2.5 | 12 |

| | | | |
|---|---|---|---|
| 162 | Predicting the sites and energies of noncovalent intermolecular interactions using local properties. *Journal of Chemical Information and Modeling*, **2012**, 52, 1061-71 | 6.1 | 12 |
| 161 | Tautomers and reference 3D-structures: the orphans of in silico drug design. *Journal of Computer-Aided Molecular Design*, **2010**, 24, 605-11 | 4.2 | 12 |
| 160 | SCRF-DFT and NMR comparison of tetracycline and 5a,6-anhydrotetracycline in solution. *Journal of Physical Chemistry B*, **2006**, 110, 24766-74 | 3.4 | 12 |
| 159 | Structures of Carbonato and Bicarbonato Complexes of Bis(1,10-phenanthroline)Zinc(II): Experiment and Theory. *European Journal of Inorganic Chemistry*, **2003**, 2003, 1562-1569 | 2.3 | 12 |
| 158 | Notizen: Das Tribenzylidenmethan-Dianion. *Chemische Berichte*, **1983**, 116, 1669-1673 | | 12 |
| 157 | Matrix interactions for radical cations: Theoretical and experimental results for the trichlorofluoromethane matrix illustrated by 19F coupling for Me2Se+ radical cations. *Chemical Physics Letters*, **1985**, 116, 79-82 | 2.5 | 12 |
| 156 | Simulation of charge transport in organic semiconductors: A time-dependent multiscale method based on nonequilibrium Green's functions. *Physical Review Materials*, **2017**, 1, | 3.2 | 12 |
| 155 | Metadynamics simulations of ligand binding to GPCRs. *Current Opinion in Structural Biology*, **2019**, 55, 129-137 | 8.1 | 11 |
| 154 | Driving forces for the self-assembly of graphene oxide on organic monolayers. *Nanoscale*, **2014**, 6, 11344-50 | 7.7 | 11 |
| 153 | The hpCADD NDDO Hamiltonian: Parametrization. *Journal of Chemical Information and Modeling*, **2017**, 57, 1907-1922 | 6.1 | 11 |
| 152 | AM1* parameters for manganese and iron. *Journal of Molecular Modeling*, **2010**, 16, 1109-26 | 2 | 11 |
| 151 | A natural bond orbital analysis of the bonding in solvated electrons within a localised electron model. *Faraday Discussions of the Chemical Society*, **1988**, 85, 365 | | 11 |
| 150 | Dissociative electron capture by chloromethane in condensed phases. *Journal of the Chemical Society Chemical Communications*, **1984**, 93 | | 11 |
| 149 | Tuning electron transfer in supramolecular nano-architectures made of fullerenes and porphyrins. *Nanoscale*, **2019**, 11, 10782-10790 | 7.7 | 10 |
| 148 | Facile C(sp(2))-C(sp(2)) bond cleavage in oxalic acid-derived radicals. *Journal of the American Chemical Society*, **2015**, 137, 3248-52 | 16.4 | 10 |
| 147 | A Three-Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. *Angewandte Chemie*, **2016**, 128, 8140-8144 | 3.6 | 10 |
| 146 | A multi-agent quantum Monte Carlo model for charge transport: Application to organic field-effect transistors. *Journal of Chemical Physics*, **2015**, 143, 044114 | 3.9 | 10 |
| 145 | Conformation and dynamics of 8-Arg-vasopressin in solution. *Journal of Molecular Modeling*, **2014**, 20, 2485 | 2 | 10 |

| | | | |
|---|---|---|---|
| 144 | Conformation-dependent QSPR models: logPOW. *Journal of Chemical Information and Modeling*, **2011**, 51, 2408-16 | 6.1 | 10 |
| 143 | Syntheses, Structures, and Reactions of Highly Strained Dihydro- and Tetrahydroacepentalene Derivatives. *Chemistry - A European Journal*, **1998**, 4, 1192-1200 | 4.8 | 10 |
| 142 | Experimental determination of the gas phase proton affinities of the conjugate base anions of 2-iodoxybenzoic acid (IBX) and 2-iodosobenzoic acid (IBA). *Organic and Biomolecular Chemistry*, **2008**, 6, 2530-3 | 3.9 | 10 |
| 141 | Fast Long-Range Adiabatic Electron Transfer in a Model Polyglycine □Helix. *Journal of the American Chemical Society*, **1999**, 121, 1379-1380 | 16.4 | 10 |
| 140 | A Combined Semiempirical MO/Neural Net Technique for Estimating 13C Chemical Shifts. *Journal of Molecular Modeling*, **1995**, 1, 22-35 | 2 | 10 |
| 139 | Catalysis of ethylene dimerization by complexation with metal radical cations: an ab initio study. *Journal of the American Chemical Society*, **1992**, 114, 506-510 | 16.4 | 10 |
| 138 | The Metallation-Elimination Reaction, II. Monocyclic Anions and Polyanions. *Chemische Berichte*, **1983**, 116, 751-760 | | 10 |
| 137 | Structure of a □-Conjugated□Dilithium Salt of an □-Keto Dianion: 1,3-Dilithiodibenzyl Ketone-(Me2NCH2CH2NMe2)2. *Angewandte Chemie International Edition in English*, **1984**, 23, 621-622 | | 10 |
| 136 | Computational approaches and sigma-hole interactions: general discussion. *Faraday Discussions*, **2017**, | 3.6 | 9 |
| 135 | Tautomeric Equilibria of Nucleobases in the Hachimoji Expanded Genetic Alphabet. *Journal of Chemical Theory and Computation*, **2020**, 16, 2766-2777 | 6.4 | 9 |
| 134 | Kohlenstoff-Nanopunkte: supramolekulare Elektronendonor-Akzeptor-Hybride mit Perylendiimiden. *Angewandte Chemie*, **2015**, 127, 8410-8415 | 3.6 | 9 |
| 133 | Direct detection of a persistent carbonyloxyl radical in the gas phase. *Angewandte Chemie - International Edition*, **2013**, 52, 9301-4 | 16.4 | 9 |
| 132 | Using Spherical Harmonic Surface Property Representations for Ligand-Based Virtual Screening. *Molecular Informatics*, **2011**, 30, 151-9 | 3.8 | 9 |
| 131 | Understanding the Reactivity of Acyl Anion Equivalents: The Epoxide Ring Opening Case. *European Journal of Organic Chemistry*, **2011**, 2011, 2548-2553 | 3.2 | 9 |
| 130 | Unprecedented triphosphinine iron interactions: Intramolecular electron transfer, reactivity round a corner, and a low-activated ring element exchange reaction. *Comptes Rendus Chimie*, **2010**, 13, 1203-1212 | 2.7 | 9 |
| 129 | Conformations and tautomers of 5a,6-anhydrotetracycline. *Journal of Physical Chemistry B*, **2005**, 109, 4279-84 | 3.4 | 9 |
| 128 | Structural changes and binding characteristics of the tetracycline-repressor binding site on induction. *Journal of Medicinal Chemistry*, **2006**, 49, 3444-7 | 8.3 | 9 |
| 127 | Molecular dynamics simulations of the tetracycline-repressor protein: the mechanism of induction. *Journal of Molecular Biology*, **2006**, 359, 1125-36 | 6.5 | 9 |

| | | | |
|---|---|---|---|
| 126 | Effect of through bond coupling and conformation on the photophysical properties of □bridged systems comprising a vinylnaphthalene donor and a dicyanovinyl acceptor. *Physical Chemistry Chemical Physics*, **2004**, 6, 3811-3823 | 3.6 | 9 |
| 125 | Ionized bicyclo[2.2.2]oct-2-ene: a twisted olefinic radical cation showing vibronic coupling. *Chemistry - A European Journal*, **2002**, 8, 1074-81 | 4.8 | 9 |
| 124 | Conformation of 6-morpholino-3-azabicyclo[3.1.0]hexane derivatives. *Journal of the Chemical Society Perkin Transactions II*, **1993**, 1901 | | 9 |
| 123 | Lithium-Ionen-katalysierte Epoxidierung durch Triplett-Disauerstoff, eine ab-initio-Studie. *Angewandte Chemie*, **1990**, 102, 697-699 | 3.6 | 9 |
| 122 | Struktur eines □-konjugierten□Dilithium-Salzes eines □-Ketodianions: 1,3-Dilithiodibenzylketon-(Me2NCH2CH2NMe2)2. *Angewandte Chemie*, **1984**, 96, 623-625 | 3.6 | 9 |
| 121 | Protonated □halogenoethyl radicals. *Journal of the Chemical Society Chemical Communications*, **1986**, 96-98 | | 9 |
| 120 | The □hole revisited. *Physical Chemistry Chemical Physics*, **2021**, 23, 16458-16468 | 3.6 | 9 |
| 119 | Conformation and Dynamics of Human Urotensin II and Urotensin Related Peptide in Aqueous Solution. *Journal of Chemical Information and Modeling*, **2017**, 57, 298-310 | 6.1 | 8 |
| 118 | Choosing the right nanoparticle size □designing novel ZnO electrode architectures for efficient dye-sensitized solar cells. *Journal of Materials Chemistry A*, **2017**, 5, 7516-7522 | 13 | 8 |
| 117 | Molecular Mechanisms of Biased and Probe-Dependent Signaling at CXC-Motif Chemokine Receptor CXCR3 Induced by Negative Allosteric Modulators. *Molecular Pharmacology*, **2018**, 93, 309-322 | 4.3 | 8 |
| 116 | A water-soluble, bay-functionalized perylenediimide derivative - correlating aggregation and excited state dynamics. *Nanoscale*, **2018**, 10, 2317-2326 | 7.7 | 8 |
| 115 | Probing charge transfer in benzodifuran-C60 dumbbell-type electron donor-acceptor conjugates: ground- and excited-state assays. *ChemPhysChem*, **2013**, 14, 2910-9 | 3.2 | 8 |
| 114 | Structure-based evolution of subtype-selective neurotensin receptor ligands. *ChemistryOpen*, **2014**, 3, 206-18 | 2.3 | 8 |
| 113 | Systematic surface scan of the most favorable interaction sites of magnesium ions with tetracycline. *Journal of Medicinal Chemistry*, **2003**, 46, 5571-4 | 8.3 | 8 |
| 112 | Ab initio calculations on electron-transfer catalysis by metal ions. *Topics in Current Chemistry*, **1996**, 1-24 | | 8 |
| 111 | Comparative MD Simulations Indicate a Dual Role for Arg1323.50 in Dopamine-Dependent D2R Activation. *PLoS ONE*, **2016**, 11, e0146612 | 3.7 | 8 |
| 110 | Can Simulations and Modeling Decipher NMR Data for Conformational Equilibria? Arginine-Vasopressin. *Journal of Chemical Information and Modeling*, **2016**, 56, 1798-807 | 6.1 | 8 |
| 109 | Binding, Thermodynamics, and Selectivity of a Non-peptide Antagonist to the Melanocortin-4 Receptor. *Frontiers in Pharmacology*, **2018**, 9, 560 | 5.6 | 7 |

| | | | |
|---|---|---|---|
| 108 | Basal Histamine H Receptor Activation: Agonist Mimicry by the Diphenylalanine Motif. *Chemistry - A European Journal*, **2019**, 25, 14613-14624 | 4.8 | 7 |
| 107 | Stability of Odd- Versus Even-Electron Gas-Phase (Quasi)Molecular Ions Derived from Pyridine-Substituted N-Heterotriangulenes. *ChemPlusChem*, **2017**, 82, 204-211 | 2.8 | 7 |
| 106 | CO and NO complexes of Fe(II) and Co(II) porphyrins. *Journal of Coordination Chemistry*, **2010**, 63, 2854-2867 | 1.7 | 7 |
| 105 | The effect of a complexed lithium cation on a norcarane-based radical clock. *Chemistry - A European Journal*, **2009**, 15, 2425-33 | 4.8 | 7 |
| 104 | Diarylpropane-1,3-dione derivatives as TetR-inducing tetracycline mimetics: Synthesis and biological investigations. *ChemBioChem*, **2009**, 10, 2924-33 | 3.8 | 7 |
| 103 | Induction of the tetracycline repressor: characterization by molecular-dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 857-66 | 4.2 | 7 |
| 102 | Electron-vibron coupling in halogenated acenaphthenequinone upon O K-edge soft x-ray absorption. *Journal of Chemical Physics*, **2011**, 135, 144301 | 3.9 | 7 |
| 101 | Some biological applications of semiempirical MO theory. *Journal of Computer - Aided Molecular Design*, **1998**, 9/11, 131-159 | | 7 |
| 100 | How does Mg(2+) affect the binding of anhydrotetracycline in the TetR protein?. *Photochemical and Photobiological Sciences*, **2004**, 3, 109-19 | 4.2 | 7 |
| 99 | Model ab Initio Studies on Methane Oxidation and Ethylene Epoxidation by the Peroxy Radical Complexed to the Lithium Cation: Are Peroxy Radical Complexes Active Intermediates in Biological Oxidations?. *The Journal of Physical Chemistry*, **1994**, 98, 13797-13803 | | 7 |
| 98 | Some cyclic C9H6 isomers and their potential trefoil aromaticity. *Tetrahedron Letters*, **1985**, 26, 1585-1588 | | 7 |
| 97 | A Feynman dispersion correction: a proof of principle for MNDO. *Journal of Molecular Modeling*, **2018**, 24, 338 | 2 | 7 |
| 96 | Interaction of Radicals with π-Holes. *Journal of Physical Chemistry A*, **2019**, 123, 3326-3333 | 2.8 | 6 |
| 95 | Multiple Binding Sites Contribute to the Mechanism of Mixed Agonistic and Positive Allosteric Modulators of the Cannabinoid CB1 Receptor. *Angewandte Chemie*, **2018**, 130, 2610-2615 | 3.6 | 6 |
| 94 | Identification of Two Distinct Sites for Antagonist and Biased Agonist Binding to the Human Chemokine Receptor CXCR3. *Angewandte Chemie*, **2016**, 128, 15503-15507 | 3.6 | 6 |
| 93 | Chromophore Multiplication To Enable Exciton Delocalization and Triplet Diffusion Following Singlet Fission in Tetrameric Pentacene. *Angewandte Chemie*, **2019**, 131, 15407-15411 | 3.6 | 6 |
| 92 | AM1 parameters for palladium and silver. *Journal of Molecular Modeling*, **2011**, 17, 2585-600 | 2 | 6 |
| 91 | Triphenylphosphonioacetylid: eine mit Isocyaniden isovalenzelektronische Spezies. *Angewandte Chemie*, **1998**, 110, 347-351 | 3.6 | 6 |

| | | | |
|---|---|---|---|
| 90 | QSAR studies using the parashift system. *SAR and QSAR in Environmental Research*, **2008**, 19, 285-302 | 3.5 | 6 |
| 89 | The ethylene/metal(0) and ethylene/metal(I) redox system: model ab initio calculations. *Journal of Molecular Modeling*, **2006**, 12, 621-9 | 2 | 6 |
| 88 | The inhibition of alpha-chymotrypsin predicted using theoretically derived molecular properties. *Journal of Molecular Graphics*, **1996**, 14, 130-5, 142 | | 6 |
| 87 | Ab Initio Simulation of Electron-Transfer Reactions: The Reaction of Alkali-Metal Atoms with Ethylene. *Zeitschrift Fur Physikalische Chemie*, **1991**, 171, 21-31 | 3.1 | 6 |
| 86 | Enhanced hyperconjugation and facile 1,2-halogen shifts in metal cation complexes of 2-halogenoalkyl radicals: an Ab initio study. *Journal of the Chemical Society Chemical Communications*, **1989**, 1082 | | 6 |
| 85 | Polymenthylenebiphenyl polyanions by metallation–elimination. *Tetrahedron Letters*, **1982**, 23, 4077-4078 | 2 | 6 |
| 84 | Resonance-Enhanced Charge Delocalization in Carbazole-Oligoyne-Oxadiazole Conjugates. *Journal of the American Chemical Society*, **2020**, 142, 18769-18781 | 16.4 | 6 |
| 83 | EMPIRE: a highly parallel semiempirical molecular orbital program: 3: Born-Oppenheimer molecular dynamics. *Journal of Molecular Modeling*, **2020**, 26, 43 | 2 | 5 |
| 82 | Cubic C8 : An Observable Allotrope of Carbon?. *ChemPhysChem*, **2015**, 16, 2165-71 | 3.2 | 5 |
| 81 | A test of improved force field parameters for urea: molecular-dynamics simulations of urea crystals. *Journal of Molecular Modeling*, **2012**, 18, 3455-66 | 2 | 5 |
| 80 | Structural Insight into the Prolyl Hydroxylase PHD2: A Molecular Dynamics and DFT Study. *European Journal of Inorganic Chemistry*, **2012**, 2012, 4973-4985 | 2.3 | 5 |
| 79 | Empirical force-field and ab initio calculations on delocalized open chain cations. *Journal of Computational Chemistry*, **1997**, 18, 28-44 | 3.5 | 5 |
| 78 | Molecular dynamics characterization of the structures and induction mechanisms of a reverse phenotype of the tetracycline receptor. *Journal of Physical Chemistry B*, **2007**, 111, 6006-14 | 3.4 | 5 |
| 77 | Excited state conformational dynamics of semiflexibly bridged electron donor-acceptor systems: a semiempirical CI-study including solvent effects. *Journal of Molecular Modeling*, **2002**, 8, 87-94 | 2 | 5 |
| 76 | New Multicentre Point Charge Models for Molecular Electrostatic Potentials from Semiempirical M0-Calculations. *Journal of Molecular Modeling*, **2000**, 6, 452-466 | 2 | 5 |
| 75 | The Chemist's Electronic Book of Orbitals **1999**, | | 5 |
| 74 | Functionalized chloroenamines in aminocyclopropane synthesis. XVII. 3,5-Cyclopiperidine-4-carboxamides with an unsubstituted 4-amino moiety. A synthetic and a conformational study. *Tetrahedron*, **1995**, 51, 3507-3520 | 2.4 | 5 |
| 73 | Lithium-Ion-Catalyzed Epoxidation by Triplet Dioxygen: An ab initio Study. *Angewandte Chemie International Edition in English*, **1990**, 29, 648-650 | | 5 |

| | | | |
|---|---|---|---|
| 72 | The e.s.r. spectra and spin distributions of benzobarrelene radical cations. *Journal of the Chemical Society Chemical Communications*, **1986**, 547-548 | | 5 |
| 71 | The methylenecycloheptatrienyl dianion. *Journal of the Chemical Society Chemical Communications*, **1976**, 798 | | 5 |
| 70 | In Silico Adoption of an Orphan Nuclear Receptor NR4A1. *PLoS ONE*, **2015**, 10, e0135246 | 3.7 | 5 |
| 69 | Semi-Empirical Mo Calculations on Enzyme Reaction Mechanisms **1997**, 307-317 | | 5 |
| 68 | A Self-Assembled Unit Comprising 12 Squaraine Dyes Built Up from Two Star-Shaped Hexasquarainyl-Benzene Molecules. *Chemistry - A European Journal*, **2019**, 25, 2831-2839 | 4.8 | 5 |
| 67 | Pre-Planarized Triphenylamine-Based Linear Mixed-Valence Charge-Transfer Systems. *Angewandte Chemie - International Edition*, **2021**, 60, 6771-6777 | 16.4 | 5 |
| 66 | An Electrically Conducting Three-Dimensional Iron-Catecholate Porous Framework. *Angewandte Chemie - International Edition*, **2021**, 60, 18065-18072 | 16.4 | 5 |
| 65 | Differences between G-Protein-Stabilized Agonist□GPCR Complexes and their Nanobody-Stabilized Equivalents. *Angewandte Chemie*, **2017**, 129, 9136-9140 | 3.6 | 4 |
| 64 | On the feasibility of reactions through the fullerene wall: a theoretical study of NH@C. *Physical Chemistry Chemical Physics*, **2017**, 19, 17199-17209 | 3.6 | 4 |
| 63 | Universal Activation Index for Class A GPCRs. *Journal of Chemical Information and Modeling*, **2019**, 59, 3938-3945 | 6.1 | 4 |
| 62 | Photoactive preorganized subphthalocyanine-based molecular tweezers for selective complexation of fullerenes. *Chemical Science*, **2020**, 11, 3448-3459 | 9.4 | 4 |
| 61 | Propagation of Holes and Electrons in Metal-Organic Frameworks. *Journal of Chemical Information and Modeling*, **2019**, 59, 5057-5064 | 6.1 | 4 |
| 60 | Intramolecular Reactivity of □Coordinated P-Heterocycles: How to Form Five-Membered Rings out of Phosphaalkynes. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2002**, 177, 1523-1527 | 1 | 4 |
| 59 | On the band gap in peptide □helices. *International Journal of Quantum Chemistry*, **2000**, 79, 120-124 | 2.1 | 4 |
| 58 | 1D Chains of Diruthenium Tetracarbonyl Sawhorse Complexes. *European Journal of Inorganic Chemistry*, **2018**, 2018, 54-61 | 2.3 | 4 |
| 57 | Charge Transport in Organic Materials: Norm-Conserving Imaginary Time Propagation with Local Ionization Energy as the External Potential. *Journal of Chemical Theory and Computation*, **2017**, 13, 6308-6316 | 6.4 | 3 |
| 56 | Synthesis of dibenzo[c,e][1,2]diazocines□ new group of eight-membered cyclic azo compounds. *Tetrahedron Letters*, **2015**, 56, 316-320 | 2 | 3 |
| 55 | Panchromatic light funneling through the synergy in hexabenzocoronene-(metallo)porphyrin-fullerene assemblies to realize the separation of charges. *Chemical Science*, **2020**, 11, 7123-7132 | 9.4 | 3 |

| | | | |
|---|---|---|---|
| 54 | Regioselective convergent synthesis of 2-arylidene thiazolo[3,2-]pyrimidines as potential anti-chikungunya agents.. *RSC Advances*, **2020**, 10, 5191-5195 | 3.7 | 3 |
| 53 | Combining Zinc Phthalocyanines, Oligo(p-Phenylenevinylenes), and Fullerenes to Impact Reorganization Energies and Attenuation Factors. *ChemPhysChem*, **2019**, 20, 2806-2815 | 3.2 | 3 |
| 52 | Simulating charge transport in flexible systems. *Perspectives in Science*, **2015**, 6, 58-65 | 0.8 | 3 |
| 51 | Direct Detection of a Persistent Carbonyloxyl Radical in the Gas Phase. *Angewandte Chemie*, **2013**, 125, 9471-9474 | 3.6 | 3 |
| 50 | Influence of electron doping on the hydrogenation of fullerene C60 : a theoretical investigation. *ChemPhysChem*, **2011**, 12, 2581-9 | 3.2 | 3 |
| 49 | Catalysis of the Quadricyclane to Norbornadiene Rearrangement by SnCl2 and CuSO4. *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2010**, 65, 347-r369 | 1 | 3 |
| 48 | The Reaction Mechanisms of Zinc Enzymes1-29 | | 3 |
| 47 | Oxidation of Disilenes: Experimental and Theoretical Studies. *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **1994**, 49, 1737-1742 | 1 | 3 |
| 46 | The stereochemistry of the dibenzylidene-ethylene dianion. *Tetrahedron Letters*, **1983**, 24, 3985-3988 | 2 | 3 |
| 45 | Alternative mechanisms for cyanide anion exchange with acetonitrile. *Tetrahedron Letters*, **1981**, 22, 2957-2960 | 2 | 3 |
| 44 | Singlet Fission in Pyrene-Fused Azaacene Dimers. *Angewandte Chemie*, **2020**, 132, 1129-1133 | 3.6 | 3 |
| 43 | How To Make Nitroaromatic Compounds Glow: Next-Generation Large X-Shaped, Centrosymmetric Diketopyrrolopyrroles. *Angewandte Chemie*, **2020**, 132, 16238-16247 | 3.6 | 3 |
| 42 | Synergy of Electrostatic and □Interactions in the Realization of Nanoscale Artificial Photosynthetic Model Systems. *Angewandte Chemie - International Edition*, **2020**, 59, 18786-18794 | 16.4 | 3 |
| 41 | DNA-Dye-Conjugates: Conformations and Spectra of Fluorescence Probes. *PLoS ONE*, **2016**, 11, e0160229 | 3.7 | 3 |
| 40 | Energy Efficient Ultrahigh Flux Separation of Oily Pollutants from Water with Superhydrophilic Nanoscale Metal□Organic Framework Architectures. *Angewandte Chemie*, **2021**, 133, 5579-5586 | 3.6 | 3 |
| 39 | The Cascade Reactions of Indigo with Propargyl Substrates for Heterocyclic and Photophysical Diversity. *Chemistry - A European Journal*, **2021**, 27, 3708-3721 | 4.8 | 3 |
| 38 | The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. *Journal of Molecular Modeling*, **2019**, 25, 156 | 2 | 2 |
| 37 | Size-Dependent Local Ordering in Melanin Aggregates and Its Implication on Optical Properties. *Journal of Physical Chemistry A*, **2019**, 123, 9403-9412 | 2.8 | 2 |

| | | | |
|---|---|---|---|
| 36 | Directional Electrostatic Bonding **2014**, 523-536 | | 2 |
| 35 | Statistical properties of spectra of chloronaphthalenes. *Journal of Mathematical Chemistry*, **2013**, 51, 857-867 | 2.1 | 2 |
| 34 | Formation of the Vilsmeier-Haack complex: the performance of different levels of theory. *Journal of Molecular Modeling*, **2011**, 17, 3209-17 | 2 | 2 |
| 33 | Multipole electrostatic potential derived atomic charges in NDDO-methods with spd-basis sets. *Journal of Molecular Modeling*, **2007**, 13, 381-92 | 2 | 2 |
| 32 | Relationships between the chemical potential and electrostatic potentials and fields at nuclei. *Molecular Physics*, **2005**, 103, 891-895 | 1.7 | 2 |
| 31 | The structure of 5a,6-anhydrotetracycline and its Mg2+ complexes in aqueous solution. *Journal of Molecular Modeling*, **2006**, 12, 953-63 | 2 | 2 |
| 30 | An authentic ortho-quinodimethane radical anion. *Journal of the Chemical Society Chemical Communications*, **1992**, 719 | | 2 |
| 29 | On the nature of the cycloheptatrienyl trianion. The decisive importance of counterion stabilization in polymetallated carbanion systems. *Journal of Organometallic Chemistry*, **1985**, 281, c17-c20 | 2.3 | 2 |
| 28 | Multipole electrostatic model for MNDO-like techniques with minimal valence spd-basis sets **2005**, 114, 159 | | 2 |
| 27 | Models of necessity. *Beilstein Journal of Organic Chemistry*, **2020**, 16, 1649-1661 | 2.5 | 2 |
| 26 | Dibenzodiazepinone-type muscarinic receptor antagonists conjugated to basic peptides: Impact of the linker moiety and unnatural amino acids on MR selectivity. *European Journal of Medicinal Chemistry*, **2021**, 213, 113159 | 6.8 | 2 |
| 25 | Comprehensive Computational Investigation of the Barton-Kellogg Reaction for Both Alkyl and Aryl Systems. *Journal of Organic Chemistry*, **2021**, 86, 7515-7528 | 4.2 | 2 |
| 24 | The Detosylation of Chiral 1,2-Bis(tosylamides). *Journal of Organic Chemistry*, **2021**, 86, 9163-9180 | 4.2 | 2 |
| 23 | A Fluorescent Benzo[g]isoquinoline-Based HIF Prolyl Hydroxylase Inhibitor for Cellular Imaging. *ChemMedChem*, **2019**, 14, 94-99 | 3.7 | 2 |
| 22 | Dispersion and polar flattening: noble gas-halogen complexes. *Journal of Molecular Modeling*, **2018**, 24, 172 | 2 | 2 |
| 21 | Accurate parametrized variational calculations of the molecular electronic polarizability by NDDO-based methods **1999**, 75, 17 | | 2 |
| 20 | Beyond the halogen bond: general discussion. *Faraday Discussions*, **2017**, 203, 227-244 | 3.6 | 1 |
| 19 | Solid-state chemistry and applications: general discussion. *Faraday Discussions*, **2017**, 203, 459-483 | 3.6 | 1 |

| | | | |
|---|---|---|---|
| 18 | Synthesis and Density Functional Theory Studies of Azirinyl and Oxiranyl Functionalized Isoindigo and (3,3')-3,3'-(ethane-1,2-diylidene)bis(indolin-2-one) Derivatives. *Molecules*, **2019**, 24, | 4.8 | 1 |
| 17 | New Types of Descriptors and Models in QSAR/QSPR **2012**, 293-305 | | 1 |
| 16 | Predictive Modeling of Molecular Properties: Can We Go beyond Interpretation? **2011**, 91-106 | | 1 |
| 15 | Investigating Protein-Protein and Protein-Ligand Interactions by Molecular Dynamics Simulations **2009**, 153-164 | | 1 |
| 14 | Modulating the dynamics of Förster resonance energy transfer and singlet fission by variable molecular spacers. *Nanoscale*, **2020**, 12, 23061-23068 | 7.7 | 1 |
| 13 | The Feynman dispersion correction for MNDO extended to F, Cl, Br and I **2019**, 25, 1 | | 1 |
| 12 | An Electrically Conducting Three-Dimensional Iron(III) Catecholate Porous Framework. *Angewandte Chemie*, **2021**, 133, 18213-18220 | 3.6 | 1 |
| 11 | Some Biological Applications of Semiempirical MO Theory **2002**, 131-159 | | 1 |
| 10 | Quantum-mechanics-based molecular interaction fields for 3D-QSAR. *Journal of Cheminformatics*, **2014**, 6, O10 | 8.6 | 0 |
| 9 | N-Terminus to Arginine Side-Chain Cyclization of Linear Peptidic Neuropeptide Y Y Receptor Ligands Results in Picomolar Binding Constants. *Journal of Medicinal Chemistry*, **2021**, 64, 16746-16769 | 8.3 | 0 |
| 8 | Synergie von elektrostatischen und π-Wechselwirkungen für die Verwirklichung von künstlichen photosynthetischen Modellsystemen auf Nano-Ebene. *Angewandte Chemie*, **2020**, 132, 18946-18955 | 3.6 | 0 |
| 7 | Stability of Odd- Versus Even-Electron Gas-Phase (Quasi)Molecular Ions Derived from Pyridine-Substituted N-Heterotriangulenes. *ChemPlusChem*, **2017**, 82, 163 | 2.8 | |
| 6 | Simulating "soft" electronics. *Journal of Cheminformatics*, **2014**, 6, O19 | 8.6 | |
| 5 | Charge Transport through Molecules: Organic Nanocables for Molecular Electronics **2011**, 157-187 | | |
| 4 | Laser-induced crosslinking of siloxanes: A semi-empirical molecular orbital study. *Angewandte Makromolekulare Chemie*, **1994**, 215, 121-128 | | |
| 3 | The formation of endo-complexes between calixarenes and amines. A reinvestigation739-747 | | |
| 2 | Redox Catalysis and Reactivity of Metalloporphyrines **2009**, 201-212 | | |
| 1 | Titelbild: An Electrically Conducting Three-Dimensional Iron(III) Catecholate Porous Framework (Angew. Chem. 33/2021). *Angewandte Chemie*, **2021**, 133, 17893-17893 | 3.6 | |