# Dennis R Salahub

List of Publications by Year
in descending order



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|---|---|---|---|
| 183 papers | 18,737 citations | 36303 51 h-index | 11607 135 g-index |
| 185 all docs | 185 docs citations | 185 times ranked | 13537 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Hexatetra-Carbon: A Novel Two-Dimensional Semiconductor Allotrope of Carbon. Computation, 2022, 10, 19. | 2.0 | 5 |
| 2 | Multiscale molecular modelling: from electronic structure to dynamics of nanosystems and beyond. Physical Chemistry Chemical Physics, 2022, 24, 9051-9081. | 2.8 | 10 |
| 3 | <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mi>b</mml:mi></mml:mrow><mml:mn and group theoretical study of properties of a carbon trimer defect in hexagonal boron nitride. Physical Review B, 2022, 105, . | 3.2 | 13 |
| 4 | Radical pairs may explain reactive oxygen species-mediated effects of hypomagnetic field on neurogenesis. PLoS Computational Biology, 2022, 18, e1010198. | 3.2 | 18 |
| 5 | A new active learning approach for adsorbateâ€“substrate structural elucidation in silico. Journal of Molecular Modeling, 2022, 28, . | 1.8 | 6 |
| 6 | XSnS<sub>3</sub> (X = Ga, In) monolayer semiconductors as photo-catalysts for water splitting: a first principles study. Journal of Materials Chemistry C, 2022, 10, 11412-11423. | 5.5 | 6 |
| 7 | Computational investigation of Ba2ZrTiO6 double perovskite for optoelectronic and thermoelectric applications. Journal of Solid State Chemistry, 2022, 314, 123385. | 2.9 | 6 |
| 8 | Radical pairs may play a role in xenon-induced general anesthesia. Scientific Reports, 2021, 11, 6287. | 3.3 | 28 |
| 9 | Global optimization ofâ€‰~â€‰1Ânm MoS2 and CaCO3 nanoparticles. Theoretical Chemistry Accounts, 2021, 140, 1. | 1.4 | 4 |
| 10 | A new active learning approach for global optimization of atomic clusters. Theoretical Chemistry Accounts, 2021, 140, 1. | 1.4 | 12 |
| 11 | Taking the multiplicity inside the loop: active learning for structural and spin multiplicity elucidation of atomic clusters. Theoretical Chemistry Accounts, 2021, 140, 1. | 1.4 | 10 |
| 12 | Preface to the special collection in honor of Fernand Spiegelman. Theoretical Chemistry Accounts, 2021, 140, 1. | 1.4 | 0 |
| 13 | Self-Consistent Auxiliary Density Perturbation Theory. Journal of Chemical Theory and Computation, 2021, 17, 6934-6946. | 5.3 | 6 |
| 14 | Lead-free, stable mixed halide double perovskites Cs2AgBiBr6 and Cs2AgBiBr6â^'xClx â€“ A detailed theoretical and experimental study. Chemical Physics, 2020, 529, 110547. | 1.9 | 38 |
| 15 | Reliability of semiempirical and DFTB methods for the global optimization of the structures of nanoclusters. Journal of Molecular Modeling, 2020, 26, 303. | 1.8 | 15 |
| 16 | Benchmarking polarizable and non-polarizable force fields for Ca2+â€“peptides against a comprehensive QM dataset. Journal of Chemical Physics, 2020, 153, 144102. | 3.0 | 9 |
| 17 | Theoretical Investigation of 6-Mercaptopurine Isomersâ€™ Adsorption on the Au(001) Surface: Revealing the Fate of Different Isomers. ACS Omega, 2020, 5, 610-618. | 3.5 | 3 |
| 18 | Molecular Simulations with in-deMon2k QM/MM, a Tutorial-Review. Molecules, 2019, 24, 1653. | 3.8 | 29 |

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| 19 | Multiscale modeling of enzymes: QMâ€cluster, QM/MM, and QM/MM/MD: A tutorial review. International Journal of Quantum Chemistry, 2018, 118, e25558. | 2.0 | 106 |
| 20 | Heterogeneous reactions of SO2 on the hematite(0001) surface. Journal of Chemical Physics, 2018, 149, 194703. | 3.0 | 10 |
| 21 | Retardation in electron dynamics simulations based on time-dependent density functional theory. European Physical Journal D, 2018, 72, 1. | 1.3 | 11 |
| 22 | Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2017, , 795-860. | | 6 |
| 23 | Electronic properties of carbon nanotubes complexed with a DNA nucleotide. Physical Chemistry Chemical Physics, 2017, 19, 7333-7342. | 2.8 | 6 |
| 24 | Effect of dispersion corrections on covalent and non-covalent interactions in DFTB calculations. Structural Chemistry, 2017, 28, 1399-1407. | 2.0 | 4 |
| 25 | Selective ion binding and transport by membrane proteins â€“ A computational perspective. Coordination Chemistry Reviews, 2017, 345, 108-136. | 18.8 | 31 |
| 26 | First-principles calculations of the structural, mechanical, electronic and bonding properties of (CrB) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 | 5.5 | 29 |
| 27 | The role of metal substitution in the promiscuity of natural and artificial carbonic anhydrases. Coordination Chemistry Reviews, 2017, 345, 73-85. | 18.8 | 11 |
| 28 | Explicit Water Molecules Play a Key Role in the Mechanism of Rhodiumâ€Substituted Human Carbonic Anhydrase. ChemCatChem, 2017, 9, 1047-1053. | 3.7 | 11 |
| 29 | Simulating Electron Dynamics in Polarizable Environments. Journal of Chemical Theory and Computation, 2017, 13, 3985-4002. | 5.3 | 41 |
| 30 | Density-functional-based tight-binding parameterization of Mo, C, H, O and Si for studying hydrogenation reactions on molybdenum carbide. Theoretical Chemistry Accounts, 2016, 135, 1. | 1.4 | 2 |
| 31 | LiCl solvation in N-methyl-acetamide (NMA) as a model for understanding Li<sup>+</sup>binding to an amide plane. Physical Chemistry Chemical Physics, 2016, 18, 4191-4200. | 2.8 | 23 |
| 32 | Application of topological analysis of the electron localization function to the complexes of molybdenum carbide nanoparticles with unsaturated hydrocarbons. Canadian Journal of Chemistry, 2016, 94, 282-292. | 1.1 | 3 |
| 33 | QM/MM Calculations with deMon2k. Molecules, 2015, 20, 4780-4812. | 3.8 | 20 |
| 34 | Representation of Ionâ€“Protein Interactions Using the Drude Polarizable Force-Field. Journal of Physical Chemistry B, 2015, 119, 9401-9416. | 2.6 | 101 |
| 35 | Progress and challenges in simulating and understanding electron transfer in proteins. Archives of Biochemistry and Biophysics, 2015, 582, 28-41. | 3.0 | 19 |
| 36 | Molybdenum Carbide Nanocatalysts at Work in the in Situ Environment: A Density Functional Tight-Binding and Quantum Mechanical/Molecular Mechanical Study. Journal of the American Chemical Society, 2015, 137, 4249-4259. | 13.7 | 28 |

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| 37 | Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. Journal of Chemical Theory and Computation, 2015, 11, 4992-5001. | 5.3 | 42 |
| 38 | Measurement and prediction of quantum coherence effects in biological processes. Physical Chemistry Chemical Physics, 2015, 17, 30772-30774. | 2.8 | 0 |
| 39 | Multiple proton relay routes in the reaction mechanism of <scp>RNAP</scp> II: Assessing the effect of structural model. Proteins: Structure, Function and Bioinformatics, 2015, 83, 268-281. | 2.6 | 4 |
| 40 | Auxiliary Density Functional Theory: From Molecules to Nanostructures. , 2015, , 1-67. | | 5 |
| 41 | Multiscale Modelling of In Situ Oil Sands Upgrading with Molybdenum Carbide Nanoparticles. Challenges and Advances in Computational Chemistry and Physics, 2015, , 415-445. | 0.6 | 2 |
| 42 | Native Defects in Î±-Mo<sub>2</sub>C: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 25517-25524. | 3.1 | 20 |
| 43 | Temperature dependence of the molecular conformations of dilauroyl phosphatidylcholine: A density functional study. International Journal of Quantum Chemistry, 2013, 113, 631-636. | 2.0 | 7 |
| 44 | Recent Progress in Density Functional Methodology for Biomolecular Modeling. Structure and Bonding, 2013, , 1-64. | 1.0 | 9 |
| 45 | Quantum Chemical Molecular Dynamics Study of the Waterâ€“Gas Shift Reaction on a Pd/MgO(100) Catalyst Surface. Journal of Physical Chemistry C, 2013, 117, 5051-5066. | 3.1 | 10 |
| 46 | Adsorption of Hexacyclic C<sub>6</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>8</sub>, C<sub>6</sub>H<sub>10</sub>, and C<sub>6</sub>H<sub>12</sub> on a Mo-Terminated Î±-Mo<sub>2</sub>C (0001) Surface. Journal of Physical Chemistry C, 2013, 117, 7069-7080. | 3.1 | 26 |
| 47 | Asymptotic Expansion for Electrostatic Embedding Integrals in QM/MM Calculations. Journal of Chemical Theory and Computation, 2012, 8, 4232-4238. | 5.3 | 15 |
| 48 | A theoretical study of the mechanism of the nucleotidyl transfer reaction catalyzed by yeast RNA polymerase II. Science China Chemistry, 2012, 55, 1887-1894. | 8.2 | 6 |
| 49 | Density functional study of benzene adsorption on the Î±-Mo2C(0001) surface. Structural Chemistry, 2012, 23, 1459-1466. | 2.0 | 16 |
| 50 | deMon2k. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 548-555. | 14.6 | 189 |
| 51 | Quantum effects in biological electron transfer. Physical Chemistry Chemical Physics, 2012, 14, 5902. | 2.8 | 31 |
| 52 | Transmission Coefficients for Chemical Reactions with Multiple States: Role of Quantum Decoherence. Journal of the American Chemical Society, 2011, 133, 3883-3894. | 13.7 | 22 |
| 53 | Spinâ€driven activation of dioxygen in various metalloenzymes and their inspired models. Journal of Computational Chemistry, 2011, 32, 1178-1182. | 3.3 | 14 |
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| 55 | Editorial: Special issue on quantum mechanical modeling of biological systems. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 1-2. | 3.6 | 11 |
| 56 | Na+, K+ and Tl+ hydration from QM/MM computations and MD simulations with a polarizable force field. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 12-20. | 3.6 | 4 |
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| 59 | Multilevel Fragment-Based Approach (MFBA): A Novel Hybrid Computational Method for the Study of Large Molecules. Journal of Chemical Theory and Computation, 2010, 6, 91-99. | 5.3 | 58 |
| 60 | A Guide to QM/MM Methodology and Applications. Advances in Quantum Chemistry, 2010, 59, 353-400. | 0.8 | 27 |
| 61 | Structural analysis of phosphatidyl choline lipids and glycerol precursors. Canadian Journal of Chemistry, 2009, 87, 1261-1267. | 1.1 | 8 |
| 62 | Exploring the molecular origin of the high selectivity of multisubunit RNA polymerases by stochastic kinetic models. Interdisciplinary Sciences, Computational Life Sciences, 2009, 1, 91-98. | 3.6 | 4 |
| 63 | Semiempirical Quantum Chemical PM6 Method Augmented by Dispersion and H-Bonding Correction Terms Reliably Describes Various Types of Noncovalent Complexes. Journal of Chemical Theory and Computation, 2009, 5, 1749-1760. | 5.3 | 312 |
| 64 | Dioxygen Activation by Mononuclear Copper Enzymes: Insights from a Tripodal Ligand Mimicking Their CuM Coordination Sphere. Inorganic Chemistry, 2009, 48, 7003-7005. | 4.0 | 11 |
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| 66 | Characterization of the active site of yeast RNA polymerase II by DFT and ReaxFF calculations. Theoretical Chemistry Accounts, 2008, 120, 479-489. | 1.4 | 41 |
| 67 | Lipid Thermodynamics: Melting is Molecular. ChemPhysChem, 2008, 9, 2321-2324. | 2.1 | 19 |
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| 81 | Negative ion photoelectron spectra simulation of V3O from a density functional study. Journal of Chemical Physics, 2003, 118, 4913-4919. | 3.0 | 19 |
| 82 | Kohnâ€“Sham density-functional study of the adsorption of acetylene and vinylidene on iron clusters, Fen/Fen+ (n=1â€“4). Journal of Chemical Physics, 2003, 119, 12279-12290. | 3.0 | 17 |
| 83 | Kohnâ€“Sham density-functional study of the formation of benzene from acetylene on iron clusters, Fe/Fen+â€‰(n=1â€“4). Journal of Chemical Physics, 2003, 119, 12291-12300. | 3.0 | 27 |
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| 88 | Kohnâ€“Sham orbitals and orbital energies: fictitious constructs but good approximations all the same. Journal of Electron Spectroscopy and Related Phenomena, 2002, 123, 345-363. | 1.7 | 113 |
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| 97 | Effect of rotation and vibration on nuclear magnetic resonance chemical shifts: Density functional theory calculations. Journal of Chemical Physics, 1999, 110, 7153-7159. | 3.0 | 26 |
| 98 | NO adsorption on Pd clusters. A density functional study. Topics in Catalysis, 1999, 9, 123-133. | 2.8 | 17 |
| 99 | Electrical and mechanical properties of distorted carbon nanotubes. Physical Review B, 1999, 60, 13824-13830. | 3.2 | 293 |
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| 104 | The effect of structural distortions on the electronic structure of carbon nanotubes. Chemical Physics Letters, 1998, 297, 45-50. | 2.6 | 130 |
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| 106 | Molecular versus Dissociative Chemisorption of Nitric Oxide on Co2and Co3(Neutral and Cationic). A Density Functional Study. Journal of Physical Chemistry A, 1998, 102, 4643-4651. | 2.5 | 14 |
| 107 | Molecular excitation energies to high-lying bound states from time-dependentâ€‰density-functionalâ€‰responseâ€‰theory: Characterizationâ€‰and correctionâ€‰ofâ€‰theâ€‰time-dependentâ€‰localâ€‰densityâ€‰approximation ionization threshold. Journal of Chemical Physics, 1998, 108, 4439-4449. | 3.0 | 4,526 |
| 108 | Embedded cluster model for chemisorption using density functional calculations: Oxygen adsorption on the Al(100) surface.. Journal of Chemical Physics, 1998, 108, 743-756. | 3.0 | 29 |

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| 109 | Density functional study of mononitrosyls of first-row transition-metal atoms. Journal of Chemical Physics, 1997, 106, 8778-8787. | 3.0 | 45 |
| 110 | Structure and properties of cobalt clusters up to the tetramer: A density-functional study. Physical Review B, 1997, 55, 10905-10921. | 3.2 | 88 |
| 111 | Reaction of a Mo Atom with H2, N2, and O2:â€‰ A Density Functional Study. Journal of Physical Chemistry A, 1997, 101, 1532-1541. | 2.5 | 22 |
| 112 | NO/Ni, NO/Ni2, and (NO)2/Ni2Interactions. A Density Functional Study. Journal of Physical Chemistry B, 1997, 101, 7464-7471. | 2.6 | 16 |
| 113 | Achieving reliability of calculations for flat potential surfaces in density functional theory: The case of Al4 and Al4+1. International Journal of Quantum Chemistry, 1997, 63, 301-311. | 2.0 | 8 |
| 114 | Investigation of Mï¿½ssbauer parameters for a set of iodine compounds using gradient-corrected density functional theory. International Journal of Quantum Chemistry, 1997, 63, 575-583. | 2.0 | 15 |
| 115 | Structure, bonding, and magnetism of small Fe , Co , and Ni clusters, n â‰ 5. Chemical Physics Letters, 1997, 271, 133-142. | 2.6 | 221 |
| 116 | The structure of triniobium dinitride from zero electron kinetic energy photoelectron spectroscopy and density functional calculations. Chemical Physics Letters, 1997, 277, 71-78. | 2.6 | 26 |
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| 120 | Comment on â€˜â€˜Density functional calculation of nuclear magnetic resonance chemical shiftsâ€™â€™ [J. Chem. Phys. 102, 2806 (1995)]. Journal of Chemical Physics, 1996, 104, 1163-1164. | 3.0 | 6 |
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| 123 | Vibrational and geometric structures of Nb3C2 and Nb3C+2 from pulsed field ionizationâ€zero electron kinetic energy photoelectron spectra and density functional calculations. Journal of Chemical Physics, 1996, 105, 10663-10671. | 3.0 | 71 |
| 124 | Calculation of ligand NMR chemical shifts in transition-metal complexes using ab initio effective-core potentials and density functional theory. Chemical Physics Letters, 1995, 235, 382-388. | 2.6 | 90 |
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| 126 | Density functional study on the reaction of CO molecules with MgO surfaces. Catalysis Today, 1995, 23, 357-364. | 4.4 | 15 |

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| 127 | Applications of the adiabatic connection method to conformational equilibria and reactions involving formic acid. Computers & Chemistry, 1995, 19, 145-154. | 1.2 | 7 |
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| 129 | The structure of Nb3O and Nb3O+ determined by pulsed field ionizationâ€“zero electron kinetic energy photoelectron spectroscopy and density functional theory. Journal of Chemical Physics, 1995, 103, 5335-5342. | 3.0 | 135 |
| 130 | A density functional study of borane and alane monoammoniate (BH3NH3,AlH3NH3). Journal of Chemical Physics, 1995, 103, 7408-7413. | 3.0 | 15 |
| 131 | All-electron local and gradient-corrected density-functional calculations ofNandipole polarizabilities forn=1â€“6. Physical Review B, 1995, 52, 2184-2200. | 3.2 | 77 |
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| 133 | Scalar Relativistic Effects on 17O NMR Chemical Shifts in Transition-Metal Oxo Complexes. An ab Initio ECP/DFT Study. Journal of the American Chemical Society, 1995, 117, 1851-1852. | 13.7 | 82 |
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| 141 | The effects of nonlocal gradient corrections in density functional calculations of hydrocarbon radical hyperfine structures. International Journal of Quantum Chemistry, 1994, 52, 879-901. | 2.0 | 51 |
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| 144 | Calculation of spinâ€”spin coupling constants using density functional theory. Chemical Physics Letters, 1994, 221, 91-99. | 2.6 | 192 |

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| 147 | Density functional study of nitrogen oxides. Journal of Chemical Physics, 1994, 100, 2910-2923. | 3.0 | 196 |
| 148 | The hyperfine structures of small radicals from density functional calculations. Journal of Chemical Physics, 1994, 100, 5066-5075. | 3.0 | 126 |
| 149 | Assessment of Kohn-Sham density-functional orbitals as approximate Dyson orbitals for the calculation of electron-momentum-spectroscopy scattering cross sections. Physical Review A, 1994, 50, 4707-4728. | 2.5 | 255 |
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