

Dimitrios A. Pantazis – List of publications

Researcher ID: **A-2434-2010** ♦ Scopus Author ID: **35248936300** ♦ ORCID: **0000-0002-2146-9065**

89. [Assessment of Double-Hybrid Density Functional Theory for Magnetic Exchange Coupling in Manganese Complexes](#)
D. A. Pantazis*
Inorganics **2019**, 7, 57. (Special Issue: *Applications of Density Functional Theory in Inorganic Chemistry*)
88. [The S₃ state of the Oxygen-Evolving Complex: Overview of Spectroscopy and XFEL Crystallography with a Critical Evaluation of Early-Onset Models for O–O Bond Formation](#)
D. A. Pantazis*
Inorganics **2019**, 7, 55. (Special Issue: *Recent Advances in Water Oxidation Catalysis*)
87. [Physical Nature of Differential Spin-State Stabilization of Carbenes by Hydrogen and Halogen Bonding: A Domain-Based Pair Natural Orbital Coupled Cluster Study](#)
R. G. Shirazi, F. Neese, **D. A. Pantazis*** and G. Bistoni
J. Phys. Chem. A **2019**, 123, 5081-5090. [**Cover article**]
86. [Proton Translocation via Tautomerization of Asn298 During the S₂–S₃ State Transition in the Oxygen-Evolving Complex of Photosystem II](#)
M. Chrysina, J. C. d. M. Silva, G. Zahariou, **D. A. Pantazis*** and N. Ioannidis
J. Phys. Chem. B **2019**, 123, 3068-3078.
85. [Multireference Approaches to Spin-State Energetics of Transition Metal Complexes Utilizing the Density Matrix Renormalization Group](#)
M. Roemelt and **D. A. Pantazis***
Adv. Theory Simul. **2019**, 1800201.
84. [Microsolvation of the Redox-Active Tyrosine-D in Photosystem II: Correlation of Energetics with EPR Spectroscopy and Oxidation-Induced Proton Transfer](#)
A. Sirohiwal, F. Neese and **D. A. Pantazis***
J. Am. Chem. Soc. **2019**, 141, 3217-3231.
83. [Meeting the Challenge of Magnetic Coupling in a Triply-Bridged Chromium Dimer: Complementary Broken-Symmetry Density Functional Theory and Multireference Density Matrix Renormalization Group](#)
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J. Chem. Theory Comput. **2019**, 15, 938-948.
82. [Applications of the Density Matrix Renormalization Group to Exchange-Coupled Transition Metal Systems](#)
V. Krewald and **D. A. Pantazis***
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81. [Missing pieces in the puzzle of biological water oxidation](#)
D. A. Pantazis*
ACS Catal. **2018**, 8, 9477-9507.
80. [Systematic high-accuracy prediction of electron affinities for biological quinones](#)
C. E. Schulz, A. K. Dutta, R. Izsák and **D. A. Pantazis***
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79. [Accurate spin-state energetics for aryl carbenes](#)
R. G. Shirazi, F. Neese and **D. A. Pantazis***
J. Chem. Theory Comput. **2018**, *14*, 4733-4746.
78. [Exchange coupling interactions from the Density Matrix Renormalization Group and *N*-Electron Valence Perturbation Theory: Application to a biomimetic mixed-valence manganese complex](#)
M. Roemelt, V. Krewald and **D. A. Pantazis***
J. Chem. Theory Comput. **2018**, *14*, 166-179.
77. [Differences in the active site of water oxidation among photosynthetic organisms](#)
M. Retegan and **D. A. Pantazis***
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76. [The first state in the catalytic cycle of the water-oxidizing enzyme: Identification of a water-derived \$\mu\$ -hydroxo bridge](#)
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