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Single Si atom supported on defective boron nitride nanosheet as a promising metal-free catalyst for N₂O reduction by CO or SO₂ molecule: A computational study. International Journal of Quantum Chemistry 2018 , 118 (16) , e25646.

A Computational Study of the Oxidation of SO₂ to SO₃ by ...

A computational study of the reactivity of rare-earth/phosphorus Lewis pairs toward polymerization of conjugated polar alkenes Y. Zhao, G. Luo, X. Xu, Z. Hou and Y. Luo, Inorg. Chem. Front., 2020, Advance Article , DOI: 10.1039/D0QI01067G If you are not the author of ...

A computational study of the reactivity of rare-earth ...

A computational study of the Fenton reaction in different pH ranges† Hsiu-Feng Lu , a Hui-Fen Chen , b Chai-Lin Kao , b Ito Chao a and Hsing-Yin Chen * b

A computational study of the Fenton reaction in different ...

A computational study of the ion gels formed by biodegradable aliphatic CBNAILS and BN nanostructures. Journal of Molecular Liquids 2019,, 112037. DOI: 10.1016/j.molliq.2019.112037. Łukasz Marcinkowski, Adam Kloskowski, Jacek Namieśnik. Nanoconfined Ionic Liquids. ...

A Computational Study of the Behavior of the Ionic Liquid ...

A computational study of the job-shop scheduling instance. David Applegate; Read more. Article. Integral infeasibility and testing total dual integrality. February 1991 · Operations Research Letters.

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A computational study of the interaction of organic surfactants with goethite α -FeO(OH) surfaces D. Santos-Carballal, Z. Du, H. E. King and N. H. de Leeuw, RSC Adv., 2016, 6, 91893 DOI: 10.1039/C6RA12377E This article is licensed ...

A computational study of the interaction of organic ...

The flow computation method and evaluation of the aerodynamic forces. The flow equations and computational method used in the present study are the same as those used in Sun and Lan . Only an outline of the method is given here. The Navier-Stokes equations are numerically solved using moving overset grids.

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In conclusion, our computational study of the Peter principle process applied to a prototypical organization with pyramidal hierarchical structure shows that the strategy of promoting the best members in the PH case induces a rapid decrease of efficiency, while it works well only if members would ideally maintain their competence at each level, a hypothesis that,

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although in agreement with common sense, seems in practice very unrealistic in the majority of real situations.

The Peter principle revisited: A computational study ...

Computational study on the mechanism and kinetics for the reaction between HO₂ and n-propyl peroxy radical. RSC Advances 2019, 9 (69), 40437-40444. DOI: 10.1039/C9RA07503H. Bo Feng, Cuihong Sun, Shaowen Zhang.

A Systematic Computational Study of the Reactions of HO₂ ...

This study aims to determine how stent design may affect in-stent hemodynamics in stented carotid arteries by means of Computational Fluid Dynamics (CFD). Methods: A robust computational method was developed to integrate detailed stent strut geometry in a patient-specific carotid artery reconstructed from medical images. Three stent designs, including two closed-cell stents and one open-cell stent, were reproduced and incorporated into the reconstructed post-stent carotid bifurcation.

A Computational Study of the Effect of Stent Design on ...

A Computational Study of the Translational Motion of Protons in Zeolite H-ZSM-5 - Volume 658 - M.E. Franke, M. Sierka, J. Sauer, U. Simon

A Computational Study of the Translational Motion of ...

A computational study of the influence of methyl substituents on competitive ring closure to α - and β -lactones. / Williams, Ian; Wilson, Philippe. In: Organic and Biomolecular Chemistry, Vol. 15, No. 34, 14.09.2017, p. 7235-7240. Research output: Contribution to journal > Article

A computational study of the influence of methyl ...

Computational study of the structure and dynamics of glycosylated SARS-CoV-2. AZoLifeSciences, viewed 14 November 2020, <https://www.azolifesciences.com/news/20201021/Computational-study-of-the-structure-and-dynamics-of-glycosylated-SARS-CoV-2.aspx>.

Computational study of the structure of SARS-CoV-2

We perform a computational study of the propagation of the oxygen concentration within a two-dimensional slice of a heterogeneous tumour region where the position and shape of the blood vessels are known. Exploiting the parameters space, we explore which effect is noticeable what concerns the formation of hypoxic zones.

Computational study of the effect of hypoxia on cancer ...

Density functional theory calculations were performed to investigate the mechanism and origins of the NHC-controlled

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selectivity of Ni-catalyzed C-H activation of arenes with vinylsilanes. The key to the selectivity is the different impacts of NHCs on the C-Si/C-C reductive elimination of the square-planar/T

The influence of NHCs on C-Si and C-C reductive ...

In The Journal of Chemical Physics, by AIP Publishing, scientists at the University of Delaware report a computational study of this nucleocapsid and show that the binding of the ssRNA allows the nucleocapsid to maintain its shape and structural integrity. Simulations of viruses are difficult because the systems are very large.

Computational study reveals how Ebola nucleocapsid ...

This approach will continue as more data emerges on the relationship between plasticity, probability of neurotransmitter release, neuronal excitations, postsynaptic potentiation and Ca^{2+}/Na^{+} levels in the perisynaptic cradle. References:[1] K. Breslin et al., "Potassium and sodium microdomains in thin astroglial processes: A computational model study," PLOS Comput.

A Computational Study of the Generalized Network Algorithms A Computational Study of the Flow of Vitreous Cutter A Computational Study of the I-35W Bridge Failure A Computational Study of the Chemistry of 3-phenylpropyl Radicals A Computational Study of the Effects of Viscoelasticity on the Interfacial Dynamics of Free Surface Displacement Flows Nanoscale Energy Transport and Harvesting A Computational Study of the Coanda Effect and Its Implementation in Web Support and Traction The Traveling Salesman Problem A Computational Study of the Dissolution of Aluminosilicate Minerals A Computational Study of the Coordination of Mg^{2+} and Ca^{2+} with Water, Hydroxide, and Phosphate A Computational Study of the Homogeneous Algorithm for Large-scale Convex Optimization A Computational Study in the Thermodynamic and Dynamic Properties of Electron Transfer Proteins A Computational Study of the 3D Flow and Performance of a Vaned Radial Diffuser Interpretation of Visual Motion Toward an Efficient Simulation of Biomineralization A Computational Study of the Impact of Mixing on Homogeneous Charge Compression Ignition A Computational Study of the Selectivity of Uracil DNA Glycosylase From Images to Surfaces Investigating the Snow Crystal A Computational Study of the Vitiation Effects on Ignition in Two-dimensional Supersonic Hydrogen/air Mixing Layer
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