

Assessment of the Perdewâ€“Burkeâ€“Ernzerhof exchange

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Citation Report

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1834	Toxic gases molecules (NH ₃ , SO ₂ and NO ₂) adsorption on GeSe monolayer with point defects engineering. <i>Chemical Physics Letters</i> , 2018, 706, 501-508.	1.2	53
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1863	Theoretical Study of Propylene Epoxidation over Cu ₂ O(111) Surface: Activity of O ²⁺ , O ⁺ , and O ₂ ⁺ Species. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21500-21513.	1.5	34
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1867	Formazanate Complexes of Hypervalent Group 14 Elements as Precursors to Electronically Stabilized Radicals. <i>Angewandte Chemie</i> , 2018, 130, 10018-10022.	1.6	6
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1932	Growth Dynamics of Millimeterâ€Sized Singleâ€Crystal Hexagonal Boron Nitride Monolayers on Secondary Recrystallized Ni (100) Substrates. <i>Advanced Materials Interfaces</i> , 2019, 6, 1901198.	1.9	20

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1960	Computational analysis of $\text{M}=\text{O}$ covalency in $\text{M}(\text{OC}_6\text{H}_5)_4$ ($\text{M} = \text{Ti}, \text{Tj}$) $\text{ET}_{0.11} \text{O}_{0.78} \text{O}_{1.14} \text{rg} \text{BT}$	1.6	26
1961	Tunable band gap of N V co-doped CaTiO_2B ($\text{CaTi}_5\text{O}_{11}$) for visible-light photocatalysis. International Journal of Hydrogen Energy, 2019, 44, 4716-4723.	3.8	12
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1963	Direct evaluation of the force constant matrix in quantum Monte Carlo. Journal of Chemical Physics, 2019, 150, 034104.	1.2	8
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1965	Carborane superhalide bases and their conjugate Brønsted-Lowry Superacids: Electron binding energies and Dyson orbitals. Chemical Physics, 2019, 521, 77-84.	0.9	9
1966	Are octahedral clusters missing on the carbon energy landscape?. Nanoscale Advances, 2019, 1, 89-93.	2.2	6
1967	Tuning the electronic properties of hexanuclear cobalt sulfide superatoms via ligand substitution. Chemical Science, 2019, 10, 1760-1766.	3.7	24
1968	Half-metal state of a Ti_2C monolayer by asymmetric surface decoration. Physical Chemistry Chemical Physics, 2019, 21, 3318-3326.	1.3	22

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1970	Aryl substituted 2,6-di(thiazol-2-yl)pyridines –excited-state characterization and potential for OLEDs. <i>Dyes and Pigments</i> , 2019, 169, 89-104.	2.0	12
1971	Electronic, magnetic, and thermodynamic properties of rhombohedral Dysprosium Manganite and discussions of effects of uniform strain, spin-orbit coupling, hole and electron doping on its electronic structures. <i>Journal of Solid State Chemistry</i> , 2019, 276, 352-360.	1.4	4
1972	Reaction pathways for surface activated rubber particles. <i>Resources, Conservation and Recycling</i> , 2019, 149, 292-300.	5.3	52
1973	Insight into the robust multiple Dirac-cones in perovskite $\text{R}_2\text{X}_2\text{M}_2\text{X}_8$ phase CuBO_3 semimetal from first-principles. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 91, 1-10.	1.3	1
1974	Relationships between NMR shifts and interaction energies in biphenyls, alkanes, azaalkanes, and oxalkanes with X^{H} and X^{H} ($X, Y = \text{C}$ or N ; $Z = \text{N}$ or O) hydrogen bonding. <i>Magnetic Resonance in Chemistry</i> , 2019, 57, 1121-1135.	1.1	8
1975	Density functional theory calculation on two-dimensional MoS_2/BiOX ($X = \text{Cl}, \text{Br}, \text{I}$) van der Waals heterostructures for photocatalytic action. <i>Applied Surface Science</i> , 2019, 492, 157-165.	3.1	65
1976	A computational investigation on the electronic and optical properties of Coronene and its Boron-Nitride and perfluorinated counterparts. <i>Journal of Physics: Conference Series</i> , 2019, 1226, 012016.	0.3	3
1977	Aromaticity of unsaturated $4\text{-}E$ heterocycles ($E = \text{N}, \text{P}, \text{As}, \text{Sb}, \text{O}, \text{S}, \text{Se}, \text{Te}$). <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18458-18466.	1.3	10
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1979	Oxoborane Formation Turns on Formazanate-Based Photoluminescence. <i>Chemistry - A European Journal</i> , 2019, 25, 11015-11019.	1.7	19
1980	The Absorption Spectrum of Guanine Based Radicals: a Comparative Computational Analysis. <i>ChemPhotoChem</i> , 2019, 3, 846-855.	1.5	9
1981	Push-pull unsymmetrical substitution in nickel(II) complexes with tetradentate N_2O_2 Schiff base ligands: synthesis, structures and linear-nonlinear optical studies. <i>Dalton Transactions</i> , 2019, 48, 11217-11234.	1.6	22
1982	Characteristics of atomic layer deposition-grown zinc oxide thin film with and without aluminum. <i>Applied Surface Science</i> , 2019, 491, 535-543.	3.1	4
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1984	Ab Initio Study of Circular Dichroism and Circularly Polarized Luminescence of Spin-Allowed and Spin-Forbidden Transitions: From Organic Ketones to Lanthanide Complexes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4140-4155.	2.3	37
1985	Delocalization Error in DFT-Predicted Extreme Long-Range Functionalization of Carbon-Doped Hexagonal Boron Nitride. <i>Journal of Physical Chemistry C</i> , 2019, 123, 15062-15070.	1.5	5
1986	Theoretical investigations of electronic and thermodynamic properties of Ce doped $\text{La}_2\text{Zr}_2\text{O}_7$ pyrochlore. <i>Materials Research Express</i> , 2019, 6, 085210.	0.8	8

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1994	Effect of mono-halogen-substitution on the electron transporting properties of perylene diimides: A density functional theory study. <i>Journal of Molecular Liquids</i> , 2019, 287, 110968.	2.3	4
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1999	Can Density Functional Theory Be Trusted for High-Order Electric Properties? The Case of Hydrogen-Bonded Complexes. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3570-3579.	2.3	21
2000	The fate of rhenium in polyaminocarboxy solution: Hourglass crystal and its speciation study. <i>Journal of Hazardous Materials</i> , 2019, 375, 78-85.	6.5	6
2001	Conjugates of thermally stable phthalocyanine J-type dimers with single-walled carbon nanotubes for enhanced optical limiting applications. <i>Optics and Laser Technology</i> , 2019, 117, 272-279.	2.2	39
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2029	<i>Ab initio</i> investigations of orthogonal ScC ₂ and ScN ₂ monolayers as promising anode materials for sodium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2019, 7, 8897-8904.	5.2	49
2030	Synthesis and Characterization of Cyclometalated NHC Platinum Complexes with Chelating Carboxylate Ligands. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2284-2290.	1.0	9
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2073	Complex Structures of Monoglucosylrutin with <i>ent</i> -Gallocatechin-3- <i>O</i> -gallate and Epigallocatechin-3- <i>O</i> -gallate in Aqueous Solutions and the Mechanism of Color Change Induced by Complexation. <i>Journal of Natural Products</i> , 2019, 82, 2-8.	1.5	3
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2093	Two-dimensional CdS/g-C ₆ N ₆ heterostructure used for visible light photocatalysis. <i>Applied Surface Science</i> , 2019, 471, 162-167.	3.1	72
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