

Improved adsorption energetics within density-functional Perdew-Burke-Ernzerhof functionals

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Citation Report

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1	Bond Activation at Monatomic Steps: NO Dissociation at Corrugated Ru(0001). Physical Review Letters, 1999, 83, 3681-3684.	2.9	183
2	Structural and electronic properties of chemisorbed oxygen on Rh(111). Physical Review B, 1999, 59, 15533-15543.	1.1	127
3	Mechanisms of self-diffusion on Pt(110). Physical Review B, 1999, 60, R5149-R5152.	1.1	45
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5	NO monomer and (NO) _x polymeric chain chemisorption on Pt{110}: Structure and energetics. Journal of Chemical Physics, 1999, 110, 12082-12088.	1.2	25
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21	Theoretical Studies of Stability and Reactivity of CH _x Species on Ni(111). Journal of Catalysis, 2000, 189, 16-30.	3.1	187
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1972	Effect of local metal microstructure on adsorption on bimetallic surfaces: Atomic nitrogen on Ni/Pt(111). <i>Journal of Chemical Physics</i> , 2013, 138, 174702.	1.2	21
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4358	Challenges for density functional theory: calculation of CO adsorption on electrocatalytically relevant metals. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9394-9406.	1.3	15
4359	Understanding trends in the activity and selectivity of bi-atom catalysts for the electrochemical reduction of carbon dioxide. <i>Journal of Materials Chemistry A</i> , 2021, 9, 8761-8771.	5.2	35
4360	Theoretical inspection of the spin-crossover [Fe(tzpy) ₂ (NCS) ₂] complex on Au(100) surface. <i>Journal of Chemical Physics</i> , 2021, 154, 034701.	1.2	6
4361	Band structure regulation in Fe-doped MgZnO by initial magnetic moments. <i>RSC Advances</i> , 2021, 11, 3209-3215.	1.7	2
4362	Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8962-9048.	1.3	47
4363	Coordination and Precipitation of Calcium Oxalate: Computation to Kinetics. <i>Crystal Growth and Design</i> , 2021, 21, 1249-1258.	1.4	4
4364	Surface reconstruction of AgPdF and AgPd nanoalloys under the formate oxidation reaction. <i>Journal of Materials Chemistry A</i> , 2021, 9, 23072-23084.	5.2	18
4365	Structural Origins of Elastic and 2D Plastic Flexibility of Molecular Crystals Investigated with Two Polymorphs of Conformationally Rigid Coumarin. <i>Chemistry of Materials</i> , 2021, 33, 1053-1060.	3.2	50
4366	A robust, freeze-resistant and highly ion conductive ionogel electrolyte towards lithium metal batteries workable at ~30 °C. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6775-6782.	1.3	12
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4369	Investigation of hydrogen bond vibrations of ice. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2021, 70, 146301.	0.2	6
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4373	Stability of Pt Skin Intermetallic Core Catalysts and Adsorption Properties for the Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2021, 125, 3527-3534.	1.5	7
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4375	Microkinetic Modeling of the CO ₂ Desorption from Supported Multifaceted Ni Catalysts. <i>Journal of Physical Chemistry C</i> , 2021, 125, 2984-3000.	1.5	20

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4395	Atomic-Step Enriched Ruthenium-Iridium Nanocrystals Anchored Homogeneously on MOF-Derived Support for Efficient and Stable Oxygen Evolution in Acidic and Neutral Media. ACS Catalysis, 2021, 11, 3402-3413.	5.5	87
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4466	Structure sensitivity of ammonia electro-oxidation on transition metal surfaces: A first-principles study. <i>Journal of Catalysis</i> , 2021, 397, 137-147.	3.1	31
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4499	Single-Step Direct Laser Writing of Multimetal Oxygen Evolution Catalysts from Liquid Precursors. <i>ACS Nano</i> , 2021, 15, 9796-9807.	7.3	11
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5111	Adsorption and Activation of CO ₂ on a Au ₁₉ Pt Subnanometer Cluster in Aqueous Environment. <i>Computational and Theoretical Chemistry</i> , 2022, , 113701.	1.1	2

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