

Molecular adsorption at Pt(111). How accurate are DFTf

Physical Chemistry Chemical Physics

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Citation Report

#	ARTICLE	IF	CITATIONS
5	Pyridine adsorption and diffusion on Pt(111) investigated with density functional theory. Journal of Chemical Physics, 2016, 144, 164112.	1.2	15
6	Electronic Structure of Iron Porphyrin Adsorbed to the Pt(111) Surface. Journal of Physical Chemistry C, 2016, 120, 29173-29181.	1.5	13
7	Systematic Error Estimation for Chemical Reaction Energies. Journal of Chemical Theory and Computation, 2016, 12, 2762-2773.	2.3	71
8	Controlling the Adsorption of Aromatic Compounds on Pt(111) with Oxygenate Substituents: From DFT to Simple Molecular Descriptors. Journal of Physical Chemistry Letters, 2016, 7, 2074-2079.	2.1	23
9	Electric Field Effects in Electrochemical CO <sub>2</sub> Reduction. ACS Catalysis, 2016, 6, 7133-7139.	5.5	411
10	Co-adsorption of O <sub>2</sub> and H <sub>2</sub> O on Al(111) surface: a vdW-DFT study. RSC Advances, 2016, 6, 79836-79843.	1.7	14
11	Energies of Formation Reactions Measured for Adsorbates on Late Transition Metal Surfaces. Journal of Physical Chemistry C, 2016, 120, 25161-25172.	1.5	63
12	C <sub>2</sub> H <sub>2</sub> -Induced Surface Restructuring of Pd-Ag Catalysts: Insights from Theoretical Modeling. Journal of Physical Chemistry C, 2016, 120, 26320-26327.	1.5	26
13	Decomposition Mechanism of Anisole on Pt(111): Combining Single-Crystal Experiments and First-Principles Calculations. ACS Catalysis, 2016, 6, 8166-8178.	5.5	34
14	Solvation free energies for periodic surfaces: comparison of implicit and explicit solvation models. Physical Chemistry Chemical Physics, 2016, 18, 31850-31861.	1.3	80
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17	Assessing a First-Principles Model of an Electrochemical Interface by Comparison with Experiment. Journal of Physical Chemistry C, 2016, 120, 5619-5623.	1.5	78
18	Perspective: On the active site model in computational catalyst screening. Journal of Chemical Physics, 2017, 146, 040901.	1.2	48
19	DFT-Based Method for More Accurate Adsorption Energies: An Adaptive Sum of Energies from RPBE and vdW Density Functionals. Journal of Physical Chemistry C, 2017, 121, 4937-4945.	1.5	80
20	Low-temperature activation of methane on the IrO <sub>2</sub> (110) surface. Science, 2017, 356, 299-303.	6.0	244
21	Adsorption and Decomposition of a Lignin Î <sup>2</sup> -O-4 Linkage Model, 2-Phenoxyethanol, on Pt(111): Combination of Experiments and First-Principles Calculations. Journal of Physical Chemistry C, 2017, 121, 9889-9900.	1.5	16
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24	Modeling the Photochromism of S-Doped Sodalites Using DFT, TD-DFT, and SAC-CI Methods. <i>Inorganic Chemistry</i> , 2017, 56, 414-423.	1.9	18
25	Ab initio coverage-dependent microkinetic modeling of benzene hydrogenation on Pd(111). <i>Catalysis Science and Technology</i> , 2017, 7, 5267-5283.	2.1	19
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42	Quantum chemical calculations to determine partitioning coefficients for HgCl <sub>2</sub> on iron-oxide aerosols. Science of the Total Environment, 2018, 636, 580-587.	3.9	9
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54	Role of Hydroxyl Groups in Low-Temperature CO Catalytic Oxidation over Zn <sub>4</sub> Si <sub>2</sub> O <sub>7</sub> (OH) <sub>2</sub> Nanowire-Supported Gold Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 25456-25466.	1.5	2
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63	Deactivation reactions on a commercial lean nox-trap - Effect of hydrocarbon nature, concentration and operation temperature. <i>Applied Catalysis A: General</i> , 2019, 585, 117178.	2.2	3
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81	Atomically Dispersed Pt <sub>1</sub> Polyoxometalate Catalysts: How Does Metal Support Interaction Affect Stability and Hydrogenation Activity?. <i>Journal of the American Chemical Society</i> , 2019, 141, 8185-8197.	6.6	147
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