Rees B Rankin

List of Publications by Year
in descending order

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34 papers	1,797 citations	430874 18 h-index	414414 32 g-index
43 all docs	43 docs citations	43 times ranked	2658 citing authors

#	Article	IF	Citations
1	Computational screening of transition metal/pâ€block hybrid electrocatalysts for CO₂ reduction. Journal of Computational Chemistry, 2020, 41, 1384-1394.	3.3	2
2	Towards quaternary alloy Auâ€“Pd catalysts for direct synthesis of hydrogen peroxide. Materials Today Energy, 2020, 16, 100399.	4.7	5
3	Similarities and differences for atomic and diatomic molecule adsorption on the B-5 type sites of the HCP(101Ì…6) surfaces of Co, Os, and Ru from DFT calculations. Heliyon, 2019, 5, e01924.	3.2	0
4	Graphene Supported Tungsten Carbide as Catalyst for Electrochemical Reduction of CO2. Catalysts, 2019, 9, 604.	3.5	12
5	Size, Composition, and Support-Doping Effects on Oxygen Reduction Activity of Platinum-Alloy and on Non-platinum Metal-Decorated-Graphene Nanocatalysts. Frontiers in Chemistry, 2019, 7, 610.	3.6	3
6	Effects of surface structure and halogen substitution on electronic charge transfer in adlayers of (BETS)2-GaCl4 on silver surfaces. Surface Science, 2019, 687, 34-40.	1.9	3
7	Computational Screening for Developing Optimal Intermetallic Transition Metal Pt-Based ORR Catalysts at the Predictive Volcano Peak. Journal of Physical Chemistry C, 2019, 123, 13236-13245.	3.1	21
8	Amino Acid Immobilization of Copper Surface Diffusion on Cu(111). Advanced Materials Interfaces, 2019, 6, 1900021.	3.7	7
9	Adsorption Energy Shifts for Oxygen and Hydroxyl on 4-atom Metal-Decorated Graphene Catalysts Via Solvation, pH, and Substrate Dopants: Effects on ORR Activity. Metals, 2019, 9, 227.	2.3	4
10	Immobilized Cu Adatoms: Amino Acid Immobilization of Copper Surface Diffusion on Cu(111) (Adv.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	3.7	0
11	Computational predictive design for metal-decorated-graphene size-specific subnanometer to nanometer ORR catalysts. Catalysis Today, 2018, 312, 105-117.	4.4	13
12	InnenrÃ¼cktitelbild: Elucidation of Pathways for NO Electroreduction on Pt(111) from First Principles (Angew. Chem. 28/2015). Angewandte Chemie, 2015, 127, 8417-8417.	2.0	0
13	Elucidation of Pathways for NO Electroreduction on Pt(111) from First Principles. Angewandte Chemie, 2015, 127, 8373-8376.	2.0	22
14	Elucidation of Pathways for NO Electroreduction on Pt(111) from First Principles. Angewandte Chemie - International Edition, 2015, 54, 8255-8258.	13.8	111
15	Chiral â€œPinwheelâ€•Heterojunctions Self-Assembled from C₆₀ and Pentacene. ACS Nano, 2013, 7, 3086-3094.	14.6	16
16	Tracking Amino Acids in Chiral Quantum Corrals. Journal of Physical Chemistry C, 2013, 117, 11757-11763.	3.1	19
17	Rational Development of Ternary Alloy Electrocatalysts. Journal of Physical Chemistry Letters, 2012, 3, 1668-1673.	4.6	130
18	Trends in Selective Hydrogen Peroxide Production on Transition Metal Surfaces from First Principles. ACS Catalysis, 2012, 2, 2664-2672.	11.2	137

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19	Trends in methanol decomposition on transition metal alloy clusters from scaling and BrÃ¸nstedâ€“Evansâ€“Polanyi relationships. Physical Chemistry Chemical Physics, 2012, 14, 8644.	2.8	30
20	Unique Electrochemical Adsorption Properties of Ptâ€Skin Surfaces. Angewandte Chemie - International Edition, 2012, 51, 3139-3142.	13.8	264
21	Exploring Computational Design of Size-Specific Subnanometer Clusters Catalysts. Topics in Catalysis, 2012, 55, 353-365.	2.8	30
22	Surface reactions of AsH3, H2Se, and H2S on the Zn2TiO4(010) surface. Surface Science, 2011, 605, 818-823.	1.9	10
23	Adsorption and Diffusion of Light Gases in ZIF-68 and ZIF-70: A Simulation Study. Journal of Physical Chemistry C, 2009, 113, 16906-16914.	3.1	126
24	The importance of chargeâ€“quadrupole interactions for H2adsorption and diffusion in CuBTC. Molecular Simulation, 2009, 35, 60-69.	2.0	39
25	Progress, Opportunities, and Challenges for Applying Atomically Detailed Modeling to Molecular Adsorption and Transport in Metalâ^'Organic Framework Materials. Industrial & Engineering Chemistry Research, 2009, 48, 2355-2371.	3.7	283
26	DFT characterization of adsorption and diffusion mechanisms of H, As, S, and Se on the zinc orthotitanate(010) surface. Surface Science, 2008, 602, 1877-1882.	1.9	2
27	Characterization of Bulk Structure in Zinc Orthotitanate: A Density Functional Theory and EXAFS Investigation. Journal of the American Ceramic Society, 2008, 91, 584-590.	3.8	17
28	Influence of Surface Reactions on Complex Hydride Reversibility. Journal of Physical Chemistry C, 2008, 112, 18270-18279.	3.1	4
29	Density functional theory calculations of the surface structure of the inverse spinel zinc orthotitanate. Journal of Physics Condensed Matter, 2008, 20, 095001.	1.8	3
30	Structures of Dense Glycine and Alanine Adlayers on Chiral Cu(3,1,17) Surfaces. Langmuir, 2006, 22, 8096-8103.	3.5	38
31	First-principles studies of chiral step reconstructions of Cu(100) by adsorbed glycine and alanine. Journal of Chemical Physics, 2006, 124, 074703.	3.0	44
32	Structure of enantiopure and racemic alanine adlayers on Cu(110). Surface Science, 2005, 574, L1-L8.	1.9	99
33	Structures of Glycine, Enantiopure Alanine, and Racemic Alanine Adlayers on Cu(110) and Cu(100) Surfaces. Journal of Physical Chemistry B, 2005, 109, 16764-16773.	2.6	101
34	Assessment of heterochiral and homochiral glycine adlayers on Cu(110) using density functional theory. Surface Science, 2004, 548, 301-308.	1.9	99