

Sally A Wasileski

List of Publications by Year in descending order

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18
papers

1,355
citations

567281

15
h-index

888059

17
g-index

18
all docs

18
docs citations

18
times ranked

1356
citing authors

#	ARTICLE	IF	CITATIONS
1	First principles reaction modeling of the electrochemical interface: Consideration and calculation of a tunable surface potential from atomic and electronic structure. <i>Physical Review B</i> , 2006, 73, .	3.2	394
2	Field-dependent chemisorption of carbon monoxide and nitric oxide on platinum-group (111) surfaces: Quantum chemical calculations compared with infrared spectroscopy at electrochemical and vacuum-based interfaces. <i>Journal of Chemical Physics</i> , 2000, 113, 4392-4407.	3.0	167
3	Electrochemical Infrared Characterization of Carbon-Supported Platinum Nanoparticles: A Benchmark Structural Comparison with Single-Crystal Electrodes and High-Nuclearity Carbonyl Clusters. <i>Journal of Physical Chemistry B</i> , 2001, 105, 9719-9725.	2.6	122
4	Field-Dependent Electrode-Chemisorbate Bonding: A Sensitivity of Vibrational Stark Effect and Binding Energetics to Nature of Surface Coordination. <i>Journal of the American Chemical Society</i> , 2002, 124, 2796-2805.	13.7	110
5	Field-Dependent Chemisorption of Carbon Monoxide on Platinum-Group (111) Surfaces: Relationships between Binding Energetics, Geometries, and Vibrational Properties as Assessed by Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2001, 105, 3518-3530.	2.6	85
6	A first-principles study of molecular oxygen dissociation at an electrode surface: a comparison of potential variation and coadsorption effects. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 3613.	2.8	76
7	Metal electrode-Chemisorbate bonding: General influence of surface bond polarization on field-dependent binding energetics and vibrational frequencies. <i>Journal of Chemical Physics</i> , 2001, 115, 8193-8203.	3.0	62
8	Periodic Trends in Electrode-Chemisorbate Bonding: Benzotrile on Platinum-Group and Other Noble Metals As Probed by Surface-Enhanced Raman Spectroscopy Combined with Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2001, 123, 12817-12825.	13.7	61
9	Potential-dependent chemisorption of carbon monoxide on platinum electrodes: new insight from quantum-chemical calculations combined with vibrational spectroscopy. <i>Journal of Electroanalytical Chemistry</i> , 2001, 500, 344-355.	3.8	59
10	From first principles to catalytic performance: tracking molecular transformations. <i>Chemical Engineering Science</i> , 2004, 59, 4703-4714.	3.8	58
11	Electronic structure models of oxygen adsorption at the solvated, electrified Pt(111) interface. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10108.	2.8	35
12	Electrode Potential-Dependent Anion Chemisorption and Surface Bond Polarization As Assessed by Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2002, 106, 4782-4788.	2.6	30
13	Some interpretations of surface vibrational spectroscopy pertinent to fuel-cell electrocatalysis. <i>Electrochimica Acta</i> , 2002, 47, 3611-3620.	5.2	27
14	Influence of Double-Layer Solvation on Local versus Macroscopic Surface Potentials on Ordered Platinum-Group Metals as Sensed by the Vibrational Stark Effect. <i>Langmuir</i> , 2001, 17, 3039-3043.	3.5	23
15	What can we learn about electrode-Chemisorbate bonding energetics from vibrational spectroscopy? An assessment from density functional theory. <i>Faraday Discussions</i> , 2002, 121, 285-300.	3.2	23
16	Vibrational spectroscopy as a probe of potential-dependent electrode-chemisorbate bonding: an assessment using finite-cluster density functional theory. <i>Journal of Electroanalytical Chemistry</i> , 2002, 524-525, 219-230.	3.8	14
17	Modeling Electrocatalytic Reaction Systems from First Principles. <i>Topics in Applied Physics</i> , 2009, , 551-574.	0.8	7
18	First-Principles Simulation of the Active Sites and Reaction Environment in Electrocatalysis. , 0, , 93-128.		2