Sally A Wasileski

List of Publications by Year
in descending order

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18	1,355	567281 15	888059 17
papers	citations	h-index	g-index

18	18	18	1356
all docs	docs citations	times ranked	citing authors

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