

Towards First-Principles Electrochemistry

By Ismaila Dabo

LAP Lambert Academic Publishing. Paperback. Condition: New. 152 pages. Dimensions: 8.7in. x 5.9in. x 0.3in.Quantum mechanical calculations are frequently used in computational surface science for predicting catalytic activities, for elucidating chemical processes, and for interpreting spectroscopic experiments. In recent years, several methods have been developed to extend the application of electronic-structure methods to surface electrochemistry. Nevertheless, computational approaches to treat electrochemical systems (e.g., fuel cells and batteries) as a function of the applied voltage had been lacking. We have developed an atomcontinuum model for the first-principles simulation of catalytic systems under electrochemical conditions. We have implemented and validated an efficient algorithm to solve the underlying nonlinear generalized Poisson equations. The approach is applied to the first-principles description of the voltage dependence of vibrational frequencies (the vibrational Stark effect) for CO on platinum electrodes, finding excellent agreement with electrochemical spectroscopic experiments and resolving previous controversies. This item ships from multiple locations. Your book may arrive from Roseburg,OR, La Vergne,TN. Paperback.



Reviews

Without doubt, this is actually the best job by any publisher. It is writter in basic phrases instead of difficult to understand. You will like the way the author publish this publication.

-- Dr. Marvin Deckow

Complete guideline for pdf lovers. It is definitely basic but shocks within the 50 percent of your ebook. I am easily could get a pleasure of studying a created publication. -- Prof. Elwyn Boehm MD

See Also

Boosting Your Pet's Self-Esteem: Or How to Have a Self-Actualized, Addiction-Free, Non-Co-Dependent Animal Companion

Macmillan General Reference. PAPERBACK. Book Condition: New. 087605680X The book is brand new. For some reason, half of the very last page in the book is missing. It in no way affects the index of the book or any of the text....

The Trouble with Trucks: First Reading Book for 3 to 5 Year Olds

Anness Publishing. Paperback. Book Condition: new. BRAND NEW, The Trouble with Trucks: First Reading Book for 3 to 5 Year Olds, Nicola Baxter, Geoff Ball, This is a super-size first reading book for 3-5 year olds, with an engaging story, colourful pictures...

Read Write Inc. Phonics: Yellow Set 5 Storybook 7 Do We Have to Keep it?

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. Tim Archbold (illustrator). 211 x 101 mm. Language: N/A. Brand New Book. These engaging Storybooks provide structured practice for children learning to read the Read Write Inc. Set1 and 2 sounds....

- ,

Games with Books : 28 of the Best Childrens Books and How to Use Them to Help Your Child Learn - From Preschool to Third Grade Book Condition: Brand New. Book Condition: Brand New.

_

Games with Books : Twenty-Eight of the Best Childrens Books and How to Use Them to Help Your Child Learn - from Preschool to Third Grade

 ${\tt Book\, Condition: Brand\, New.\, Book\, Condition: Brand\, New.}$

-

Index to the Classified Subject Catalogue of the Buffalo Library; The Whole System Being Adopted from the Classification and Subject Index of Mr. Melvil Dewey, with Some Modifications .

Rarebooksclub.com, United States, 2013. Paperback. Book Condition: New. 246 x 189 mm. Language: English. Brand New Book ***** Print on Demand *****. This historic book may have numerous typos and missing text. Purchasers can usually download a free scanned copy of the...