Development of theoretical surface spectral apparatus

2007 Fiscal Year Final Research Report Summary

DEVELOPMENT OF THEORETICAL SURFACE SPECTRAL APPARATUS

Research Project

Project/Area Number

18550013

Research Category

Grant-in-Aid for Scientific Research (C)

Allocation Type

Single-year Grants

Section

一般

Research Field

Physical chemistry

Research Institution

Kanazawa University

Principal Investigator

ENDO Kazunaka Kanazawa University, Graduate School of Natural Science and Technology, Professor (20293334)

Co-Investigator(Kenkyū-buntansha)

IDA Tomonori Kanazawa University, Graduate School of Natural Science and Technology, ASSISTANT (30345607)
MIZUNO Mtohiro Kanazawa University, Graduate School of Natural Science and Technology, ASSOC, PROFESSOR (70251915)

Project Period (FY)

2006 – 2007

Keywords

ELECTRON SPECTRUM / MASS SPECTROMETRY / SOLID NMR / MOLECULAR DYNAMICS / MOLECULAR ORBITAL METHOD / DENSITY FUNCTIONAL METHOD

Research Abstract

We considered from two theoretical viewpoints of both (A) time-independent and (B) time-dependent Hamiltonian for the development of theoretical surface spectral apparatus, in order to simulate electron spectra of substances by surface scientific instruments, and to gain the mass spectra by MS and static or TOF SIMS, respectively.
In (A), six kinds of spectral analyses were performed in the following way; (1) X-Ray Photoelectron and Carbon Kα Emission measurements and calculations of O-, CO-, N-, and S-containing Substances (The combined analysis of valence XPS and carbon Ka XES for PEO, PVA, PVME, PVMK, PET, P4VP, PAO, PPS polymers was performed to determine the individual contributions from pσ-, and pπ-bonding molecular orbitals of the polymers by DFT calculations. We calculated all CEBEs of the model molecules using the ΔE_ks approach. Our simulated Cls photoelectron and C Kα emission spectra are in good agreement with our measurements.), (2)Electronic structure of a Mn_12 molecular ⋯▾ More

Research Products (50 results)

All | 2008 | 2007 | 2006

All | Journal Article (28 results) (of which Peer Reviewed: 16 results) | Presentation (20 results) | Book (2 results)

[Journal Article] Dynamics of[Zn(D_2O)_6]^<2+>in[Zn(D_2O)_6][SiF_6]crystal as studied by 1D,2D spectra and spin-lattice relaxation time of 2D NMR, 2008

[Journal Article] Fragment Distribution of Thermal Decomposition for PS and PET with QMD Calculations by Considering the Excited and Charged Model Molecules 2008

[Journal Article] Fragment Distribution of Thermal Decomposition for Lignin Monomer by QMD Calculations using the Excited and Charged Model Molecules 2008

[Journal Article] Simulation of SIMS for monomer and dimer of lignin under the assumption of thermal decomposition using QMD method 2008

[Journal Article] Conformation and Molecular Dynamics of Single Polystyrene Chain Confined in Cooordination Nanospace. 2008

[Journal Article] Theoretical analysis of Auger electron spectra of 2nd periodic element containing substances 2008

[Journal Article] XPS Spectral Simulation of Chitosan in Thermal Decomposition Process 2008

[Journal Article] X-Ray Photoelectron Spectral Analysis for Carbon Allotropes 2008

[Journal Article] 表面・界面分析法によるポリマーのスペクトル解析-実測スペクトルとシミュレーションから何がわかるか- 2008

[Journal Article] Molecular dynamics in paramagnetic materials as studied by magic-angle spinning 2H NMR spectra 2008

[Journal Article] Dynamics of [Zn(D_2O)_6]2+in [Zn(D_2O)_6][SiF_6] crystal as studied by 1D, 2D spectra and spin-lattice relaxation time of 2D NMR 2008

[Journal Article] Fragment Distribution of Thermal Decomposition for PS and PET with QMD Calculations by Considering the Excited and Charged Model Molecules 2008

[Journal Article] Fragment Distribution of Thermal Decomposition for Lignin Monomer by QMD Calculations using the Excited and Charged Model Molecules 2008

[Journal Article] Simulation of SIMS for monomer and dimer of lignin under the assumption of thermal decomposition using QMD method 2008

[Journal Article] Theoretica analysis of Auger electron spectra of 2nd periodic element containing substances 2008

[Journal Article] XPS Spectral Simulation of Chitosan in Thermal Decomposition Process 2008

[Journal Article] Electronic structure of a Mn_<12> molecular magnet: Theory and experiment 2007

[Journal Article] X-Ray Photoelectron and Carbon Kα Emission measurements and calculations of O-, CO-,N-, and S-containing Substances 2007

[Journal Article] Two-dimensional wavepacket dynamics with quantum hydrodynamics 2007

[Journal Article] Molecular dynamics in paramagnetic materials as studied by magic-angle spinning 2H NMR spectra 2007

[Journal Article] X-Ray Photoelectron and Carbon Kα Emission Measurements and Calculations of O-, CO-, N-, and S-containing Substances 2007

[Journal Article] Two-dimensional wavepacket dynamics with quantum hydrodynamics 2007

[Journal Article] Simulation of resonant X-ray emission spectra of ethylene and benzene molecules 2006

[Journal Article] Local Structure Analysis of Smoky and Colorless Topaz Using Single Crystal^<27> Al NMR 2006

[Journal Article] Immobilization of Sodium Ions on the Pore Surface of a Porous Coordination Polymer 2006

[Journal Article] Immobiliza-tion of Sodium Ions on the Pore Surface of a Porous Coordination Polymer 2006

[Journal Article] Simulation of resonant X-ray emission spectra of ethylene and benzene molecules 2006

[Journal Article] Dynamic Motion of Building Blocks in Porous Coordination Polymer 2006

[Presentation] Theoretical Auger spectra of molecule by two-electron propagator method 2008

[Presentation] Wavepacket dynamics simulation of nonadiabatic trajectory by quantum trajectory method 2008

[Presentation] Theoretical Auger spectra of molecule by two-electron propagator method 2008

[Presentation] Wavepacket dynamics simulation of nonadiabatic trajectory by quantum trajectory method 2008

[Presentation] Theoretical analysis of Auger electron spectra of 2nd periodic element containing substances 2007

[Presentation] XPS Spectral Simulation of Chitosan in Thermal Decomposition Process 2007

[Presentation] X-Ray Photoelectron Spectral Analysis for Carbon Allotropes 2007

[Presentation] Theoretical analysis of Auger electron spectra of 2nd periodic element containing substances 2007

[Presentation] XPS Spectral Simulation of Chitosan in Thermal Decomposition Process 2007

[Presentation] X-Ray Photoelectron Spectral Analysis for Carbon Allotropes 2007

[Presentation] Fragment Distribution of Thermal Decomposition for PS and PET with QMD Calculations by Considering the Excited and Charged Model Molecules 2007

[Presentation] Fragment Distribution of Thermal Decomposition for PS and PET with QMD Calculations by Considering the Excited and Charged Model Molecules 2007

[Presentation] Simulation of SIMS for monomer and dimer of lignin under the assumption of thermal decomposition using QMD method 2007

[Presentation] Fragment Distribution of Thermal Decomposition for Lignin Monomer by QMD Calculation using the Excited and Charged Model Molecules 2007

[Presentation] Simulation of SIMS for monomer and dimer of lignin under the assumption of thermal decomposition using QMD method 2007

[Presentation] Fragment Distribution of Thermal Decomposition for Lignin Monomer by QMD Calculations using the Excited and Charged Model Molecules 2007

[Presentation] Simulations of thermal decomposition for carbon allotrope molecules 2006

[Presentation] Simulation of SIMS and XPS for polymers **2006**

[Presentation] Simulations of thermal decomposition for carbon allotrope molecules by a quantum molecular dynamics method **2006**

[Presentation] Simlations of SIMS and XPS for polymers **2006**

[Book] 日本表面分析科学会編[表面分析技術選書 計算シミュレーションと分析データ解析]第二部分析データ解析のための計算シミュレーション2.構造解析法 2.1 非生体材料2.1.2 NMR **2008**

[Book] 日本表面分析科学会編[表面分析技術選書 計算シミュレーションと分析データ解析]第二部分析データ解析のための計算シミュレーション3章電子分光法3.1化学シフト **2008**

URL: https://kaken.nii.ac.jp/report/KAKENHI-PROJECT-18550013/185500132007kenkyu_seika_hokoku_

Published: 2010-02-03