2014/2/8 NCRS Forum / GA Lecture Series

FY2013 The 2nd Novel Carbon Resource Sciences (NCRS) Forum / Green Asia (GA) Lecture Series

Forum I (Effective Energy Utilization) / II (Energy Saving) / III (Asian Environment)

Date: Saturday, 8 February, 13:30-16:50

Place: Room 303, 3rd Floor, C-Cube, Chikushi Campus, Kyushu University

Theme: Computational Chemistry, Analytical Chemistry and Electrochemistry

13:30-14:30	First-Principles Calculation: Can It Save the Earth? (PDF file) Tamio OGUCHI Professor, Institute of Scientific and Industrial Research, Osaka University
14:40-15:40	What is an EXAFS? Hisanobu WAKITA Professor Extraordinary, Synchrotron light Application Center, Saga University
15:50-16:50	Q & A, Discussion with students

Tamio Oguchi Professor, Institute of Scientific and Industrial Research (ISIR), Osaka U; PhD in Physics 1983 at U of Tokyo (supervisor: Prof. K. Terakura); Post Doc. 1983–1986 at Northwestern U (Prof. A. J. Freeman); Researcher 1986–1993 at National Research Institute for Metals; Associate Professor 1993–1996 at Hiroshima U; Professor 1996–2010 at Hiroshima U; Professor 2010–present at Osaka U; Condensed Matter Physics Theory; Tel: +81-6-6879-8537, Fax: +81-6-6879-8539, E-mail: oguchi@sanken.osaka-u.ac.jp.

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1993　広島大学理学部物性学科　助教授
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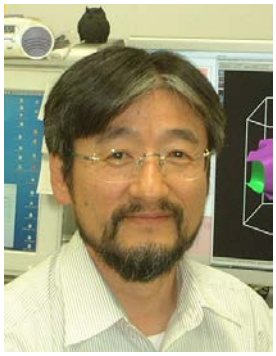
1998　広島大学大学院先端物質科学研究科量子物質科学専攻　教授
2010　大阪大学産業科学研究所　教授　現在に至る



First-Principles Calculation: Can It Save the Earth?

Professor Tamio OGUCHI

Institute of Scientific and Industrial Research, Osaka University

Abstract

Since the proposal of density functional theory (DFT) in 1964, first-principles electronic-structure calculation has become a powerful and indispensable tool for various problems in the fields of physics and chemistry for molecules and condensed matter systems. Growing progress of the DFT calculation has been accelerated by a large number of methodological developments and rapid advance in computer performance. Main characteristic features of the first-principles DFT approach are twofold: *General-purpose*: the methods do not depend on materials systems and properties we intend to study; *Non-empirical*: the methods do not require any experimental parameters as input except for fundamental physical quantities such as electron mass, Planck constant, and elementary charge. Starting from full Hamiltonian for a system containing electrons and nuclei, problems are reduced to practically solvable Kohn-Sham equations under Born-Oppenheimer (BO) and local-density approximations. The basic input parameters for the equations are only the atomic numbers and positions of the constituent atoms. By numerically solving them, total energy (BO potential) that governs the nucleic motion can be computed to determine the stable structure and to estimate the heat of formation or reaction between different structures and phases. In addition, several kinds of observables can be calculated with an extra load of computation to be directly compared with relevant experiments. The most important implication of the DFT calculation is that electronic nature and mechanisms governing physical phenomena and properties can be disclosed. In this talk, I will briefly explain fundamental aspects and typical applications of the state-of-the-art DFT calculations and present some results of our recent studies on energy materials, especially hydrogen storage materials and cathode materials for sodium secondary batteries.

第一原理計算：それは地球を救えるか？

小口多美夫

大阪大学産業科学研究所　教授

概要

1964年の密度汎関数理論(DFT)の提案以降、第一原理電子状態計算は分子系・凝縮系の物理・化学の分野における様々な問題に対して強力かつ不可欠な研究手法となってきた。DFT計算の発展は多くの方法論の開発と計算機能力の急速な進展によって加速されてきている。第一原理DFT手法の特長として次の2点が挙げられる。汎用性：手法が適用される物質系や性質に依存していない。非経験性：方法が基本的な物理量（電子質量、プランク定数、電荷素量）を除いて実験的パラメータをその入力として要求しない。電子と原子核を含む系の全ハミルトニアンから出発して、ボルン・オッペンハイマー(BO)近似と局所密度近似の下に問題は実際に解くことのできるコーン・シャム方程式に還元される。その方程式の基本的な入力パラメータは構成原子の原子番号と位置だけである。それを数値的に解くことによって原子の運動を支配する全エネルギー（BOポテンシャル）が得られ、安定構造を決定し、異なる構造や相間の生成・反応エネルギーを見積もることができる。加えて、付加的な計算によって様々な物理量が求められ、関係する実験との直接的な比較が行われる。DFT計算結果の最も重要な点は物理現象や性質を支配する電子論的本質や機構が明らかにされることである。本講演では、まず最先端のDFT計算の基礎的事項と典型的な応用例を簡単に説明し、エネルギー関連材料、具体的には水素吸蔵材料とNa二次電池正極材料に関する最近の我々の研究成果を紹介する。

2014/2/8(sat) at Kyushu University

Lecture for EXAFS by Hisanobu Wakita

Hisanobu Wakita, Personal History
March 1969 Master of Science from Master Course in Chemistry, Graduate School of Science, Tokyo University of Education
March 1972 Doctor of Science from Doctoral Course in Chemistry, Graduate School of Science, Tokyo University of Education
April 1972 Lecturer in Chemistry at Fukuoka University
April 1975 Associate Professor in Chemistry at Fukuoka University
October 1985 Professor in Chemistry at Fukuoka University
April 2013 Emeritus Professor at Fukuoka University
April 2013 Part-time lecturer at Fukuoka University
April 2013 Professor Extraordinary at Synchrotron light Application Center of Saga University

Abstract of the lecture

What is an EXAFS ?　by Hisanobu Wakita

EXAFS is a kind of X-ray Absorption Spectrometry. The EXAFS oscillation appears as modulations at the absorption edge of X-rays in materials, and derives from the Kronig region with the local ordering of atoms in materials. Depending on the development of the analysis technique for the EXAFS oscillation and measuring facilities using by Synchrotron light, the EXAFS method has been progressed remarkably. The items of this lecture are:
1 What is an EXAFS oscillation ?　Origin the modulation at absorption edge of X-rays
2 How to analyze the oscillation　EXAFS formula and how to analyze the formula
3 Application examples　Crystals, amorphous solid, solution, and biomaterial samples
4 Future view in this method　Quick EXAFS and time-resolved EXAFS
This lecture is given by using Microsoft power point and delivered pictures and tables. If you hope to study this lecture, prepare what is X-rays and how to analyze sign functions.