

Selected Novel Technologies for Licensing

MRS Fall 2011

Carbon Related Materials

 Graphene, Bucky Gel, Bucky Ball, Carbon Nanotube, Carbon Nanohorn, Carbon Nanowall etc.

Other Innovative Technologies

 Isotopomer, Dendrimer, Optical Catalyst, 12CaO·7Al₂O₃, MRDFT etc.



Japan Science and Technology Agency

Carbon Related Materials



Fabrication of Graphene Using Liquid Ga and its Electrical Properties

1. Fabrication of Graphene film

- Prof. Jun-ichi FUJITA (University of Tsukuba)
- 20nm amorphous-Carbon film is deposited on the substrate.
- Liquid Ga is put on the amorphous carbon film and is annealed at 1000 for 30 min under 5 x 10⁻⁴Pa.
- Ga droplet is removed by soaking it in dilute HCI.



10 nm

2. Feature of Our Method

Method	Mechanical Delamination	High temperature anneal of carbon film on SiC crystal substrate	High temperature CVD on metal crystal substrate	Our method
Example	K. S. Novoselov et al. PNAS 102 (2005) 10451.	W. Norinatsuset al.Chem. Phys. Lett. 468 (2009) 52.	J. Coraux et al. Nano Lett. 8 (2008) 565.	J. Fujita et al. J. Appl. Phys. Lett. 49, 06GC01 (2010)
Fabrication Temperature	-	1500	900~1000	900~1000
Large area fabrication	x			
Electron mobility				(improved)
High volume production	XX	x		
Device fabrication	x			
Others		Expensive SiC crystal		•Flexible substrate is available •No transcription

4. a-Carbon Thickness Dependencies of Channel **Conductance and Moduration ratio**



Patent No. : PCT/JP2010/054602 Patent owner contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486 e-mail: license@jst.go.jp

3. Trial of Graphene Transistor



Carbon Nanohorn

Prof. Sumio IIJIMA (Meijo University) Prof. emeritus Hidekazu TOUHARA (Shinshu University)

Fabrication of Carbon Nanohorn

Carbon nanohorns are manufactured by the CO₂ laser ablation of carbon.



Carbon Nanohorn



2~4 nm

Application

- Electrical conductors
- Drug delivery
- Li⁺ capacitor battery
- Metal absorber
- Gas absorber ex. <u>Fluorine Gas</u>

Fluorine (F₂) storage nano-cylinder

This research was sponsored by NEDO (New Energy & Industrial Technology Development Organization.

- Carbon nanohorns (CNHs) indicate the behavior of F₂ adsorption- desorption.
- Hole-opend CNHs is one of the best candidate as a nano-cylinder for F₂ storage which adsorbs 100 wt% F₂/CNH and releases almost 100% of adsorbed F₂.



CNHs Fabrication Patent owner contact

 Patent license is available.
 Patent No. : JP4394383,US10/560808,EP4745618.1,CN200480016853.9; JP3479889,US10/483796,EP2746051.8,CN200202814122.9
 Patent owner contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486, e-mail: license@jst.go.jp



• F₂ purity more than 99%

- Repeated use of CNHs
- F₂ release on heating under reduced pressure

Carbon Nanotubes Encounter Ionic Liquids to create New Soft Materials



Patent license is available.

Patent No. : US7531114, JP3676337, KR627184, CN200380101950.3, (EP1555242) Patent owner contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486, e-mail: license@jst.go.jp

Cycloparaphenylene (CPP)

Prof. Kenichiro ITAMI (Nagoya University)

<u>1. CPP Molecular Structure</u>

- Despite the structural simplicity and beautiful structure of CPP, no successful synthesis had been reported at the inception of our work.
- CPP has a potential precursors in the preparation of structurally uniform armchair or carbon nano-tube.



2. Synthesis of CPP

- Synthesis strategies are ;
 - 1) Using linear (arene) & bent (cyclohexane) units
 - 2) Using Pd-catalyzed Suzuki-Miyaura cross-coupling reactions to connect both linear and bent units
 - 3) Using acid for final transformation to CPP
- Our success in synthesis of CPP (n=9,12,14,15,16)





Carbon Nano Tube



3. Patent Status & Patent contact

Patent license is available.

Patent No. : PCT/JP2011/052948, PCT/JP2011/055423 Patent contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486, e-mail: license@jst.go.jp

Water Soluble Fullerenes for Biomaterials

1. Solubilization of Fullerenes by water soluble block copolymers

University of Tsukuba



Patent No. :WO2005/035651 Patent owner contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486 e-mail: license@jst.go.jp

Formation of Fullerene Nanostructures from Metastable Metal Oxides on a-C thin film by Electron Beam Irradiation



(a) Os

(b)540s

00s (d)1260s HRTEM images

2. Fullerene Composite and its tensile strength reinforcement

(c) 900s

Fullerene Composite reinforces the tensile strength of C60 drastically



e)1800s

(f) 2100s

(g) 2460s

Excellent Mechanical Properties of Hybridized Carbon Nano-composite Thin Films

1. Fabrication of Hybridized Carbon Films



Column regions : d=1.8 g/cm3 Inter-column regions : d=1.6 g/cm3

50.00 nm

Dr. Eiji IWAMURA (Arakawa Chemical Ind. Ltd.)

Sputtering method is used under the conditions of both low temperature of substrate and high pressure of atmosphere gas for fabrication of network structures consisting of columns and inter-column regions in a-C films.

Hybridized a-C film : Thickness: 500 nm Sputter deposited on Si wafer Substrate : Room temp. Ar+CH₄ gas pressure: 4Pa

2. Structural Modification by low-energy EB Irradiation

After EB irradiation



3. Mechanical Properties of EB irradiated film

EB irradiated film shows not only superior wear resistance but high elasticity.



Film hardness : Nanoidentation test

Micro-wear resistance test

L: Total scan length~0.27cm



4. Patent status & Patent owner contact

Patent license is available. Patent No. :WO2005/083144 Patent owner contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486 e-mail: license@jst.go.jp

Carbon Nanowall Substrate for Matrix-free Laser Desorption/Ionization Mass Spectrometry

Prof. Masaru HORI (Nagoya University) Dr. Hiroaki SATO (AIST)

Carbon nanowall substrate, which is fabricated by RI-PECVD (Radical Injection Plasma-enhanced CVD), is very useful for matrix-free laser desorption ionization-mass spectrometry in which mass spectra can be easily observed without obstructive peaks and with good reproducibility.

1. Fabrication of Carbon Nanowall

RI-PECVD Equipment



Carbon Nanowall Substrate ; Low cost & Wide variation



 O_2 : 0 sccm (0%) Thickness: 1200 nm Growth rate: 60 nm/min

2 sccm (1.3%) 760 nm 19 nm/min

5 sccm (3.2%) 890 nm 22 nm/min

2. Mass Spectra using Cabon Nanowall



3. Patent status & Patent contact

Patent license is available. : JP2009-183797, PCT application Patent No. Patent contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486, e-mail: license@jst.go.jp

MALDI-Mass Spectrometry

Prof. Yoshito TOBE (Osaka University)

<u>1. Synthesis of Substituted Hexaethynylbenzenes</u></u>

 Highly efficient synthesis method of differentially substituted hexaethynylbenzens from chloroiodobenzenes.



2. Emission Spectra

 Elongated -conjugated compounds show red-shift emission spectra, which indicate small band gap.





4. Patent status & Patent owner contact

Patent license is available.
 Patent No. : US6953871, JP4150168
 Patent owner contact: Masaru OZAKI (JST)
 Tel:+81-3-5214-8486, e-mail: license@jst.go.jp

Diamond DNA Sensor

Dr. Hiroshi KAWARADA (Waseda University)

1. Fast, easy, and lowcost label-free detection can be obtained by FET type sensor.



Nanographite Structure/Metal Nanoparticle Composite

Kiyotaka SHIBA (JFCR), Kenichi SANO (RIKEN) and Kenji IWAHORI (NAIST)

The ferritin molecule displaying carbon nanohorn binding peptide-1 (NHBP-1) on its surface makes it possible to construct nanographite-metal nanoparticle composite by filling the interior of ferritin with metal dots.

1. Construction NHBP-1 displaying ferritin



Ferritin

Fig. 1: NHBP-1 is the peptide aptamer that binds to the surface of nanographite. By fusing the peptide to the N-terminal of ferritin subunit, we can endow ferritin with graphite binding ability. Ferritin can be deposited with various metal nanodots in its inner space.

Kase D, Kulp III JL, Yudasaka M, Evans JS, lijima S, Langmuir 20(20): 8939-8941 (2004)

Sano K, Ajima K, Iwahori K, Yudasaka M, Iijima S, Yamashita I, Shiba K. Endowing a ferritin-like cage protein with high affinity and selectivity for certain inorganic materials Small 1 (8-9): 826-832 (2005)

2. Making nanoelectronic devices using NHBP-1 displaying ferritin filled with metal dots.







CNT + Dps Random network



CNT + Dps parallel network

Fig. 2: Recently, Yamashita et al. at NAIST are using this technology to make novel type of electronic devices, in which they fused NHBP-1 to bacterial ferritin, Dps, and prepared the carbon nanotube (CNT)-semiconductor nanodots composites for novel type of electronic devices (personal communication).

3. Growing giant two-dimensional NHBP-1 displaying ferritin filled with metal dots.



Fig. 3: NHBP-1 has a self-assembling ability that makes it possible to grow two-dimensional array of metalcontaining ferritin.

Matsui T, Matsukawa N, Iwahori K, Sano K, Shiba K, Yamashita I. Realizing a two-dimensional ordered array of ferritin molecules directly on a solid surface utilizing carbonaceous materials-affinity Langmuir 23(4): 1615 -1618 (2007)

Ikezoe Y, Kumashiro Y, Tamada K, Matsui T, Yamashita I, Shiba K, Hara M. Giant growth of two-dimensional crystal of protein molecu from a three-phase contact line. Langmuir 24(22): 12836-12841 (2008)

4. Patent status & Patent owner contact

Patent license is available. : US-2010-0029910-A1 Patent No. Patent owner contact: Yoshihiro Murai (JST) Tel:+81-3-5214-8486 e-mail:license@jst.go.jp

Other Innovative Technologies



High-water-content Hydrogel

1. New Aqua Material

- Mostly water (>95% Water ; <0.2% Organic)</p>
- Easily preparable
- Disposable (Environment friendly)
- Self-standing (Transportable)
- Self-healable
- Adhesive
- Transparent
- Non-flammable
- Capable of containing bioactivities

2. Preparation of New Agua Material

Aqua material can readily be prepared by mixing three components in water at RT.





3. Properties of New Agua Material Moldable, Self-standing, & Transparent



4. Patent status & Patent owner contact

Patent license is available. : PCT/JP2010/004267, JP2009-156670 Patent No. **Apply country : Worldwide** Patent owner contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486, e-mail: license@jst.go.jp

Comparison of Hydrogels

	Water Content	Content of Organic Components	Mechanical Strength	Required Skill (time)	Selfheoloble	Resistant to Organic Solvents
Double Network Hydrogel	90%	10%	17 MPa	Very High [2 days]	NO	YES
Nanocomposite Hydrogel	89%	8%	1 MPo	Very High (20 h)	NO	YES
Aqua Material (Our Hydrogel)	98% 95%	0.2%	0.1 MPs 0.5 MPs	Just Mixing (3 soc)	3 sec (100%)	YES
Oligoelectrolyte Hydrogel	97%	3%	0.01 MRa	Low (30 min)	10 sec (100%)	NO
Oligopeptide Hydrogel	995	195	0.00017 MPs	Low (overnight)	24 h (100%)	NO

Application

- Regenerated material for bone, cartilage etc.
- ·Buffer material for sports shoes etc.
- ·Alternative rubber, plastic etc.
- ·Fire extinguishant etc
-

Prof. Takuzo AIDA (Tokyo University)



Electro-conductive & Transparent Nano-porous Compound C12A7

Prof. Hideo HOSONO (Tokyo Institute of Technology)

1. Novel Compound 12CaO · 7Al₂O₃ (i.e.C12A7)

- C12A7 is composed of materials of alumina cements, and has 6 cages with an inner free space of 0.4nm of which only one cage is filled by O²⁻. These 80% cages are free spaces.
- The oxide ions can be replaced by various anions such as O⁻, H⁻, OH⁻, e⁻ etc and show very interesting functions.



2. Electride C12A7: e⁻

Conductivity of C12A7: e⁻



 Cathode ray emission from C12A7: e⁻



Reduction reaction using C12A7: e⁻



3. Small work function of C12A7: e-



4. Patent status & Patent owner contact

Patent license is available.

Patent No. :US6818192,7462334.7235225,7507289,7465433, EP1717217, JP4147324,4219821,4245608, TW283234 etc Patent owner contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486 e-mail: license@jst.go.jp

Photocatalyst Releasing Hydrogen from Water

Prof. Kazunari DOMEN (University of Tokyo)

1. Direct Splitting of Water by Visible Light

New catalyst is a solid solution of Ga-Zn-O (ex.Ga_{0.7}Zn_{0.3}N_{0.7}O_{0.3}) modified with nano-particles of Rh-Cr oxide



High resolution TEM image Cr oxide (shell) Rh (core)

Cr oxide/Rh/GaN:ZnO after Cr³⁺ deposition

The quantum efficiency of water splitting by visible light is about 5% at 410nm





2. Improved Method for Higher Quantum Efficiency

 Two step excitation system on water splitting under visible light



3. Patent status & Patent owner contact

Patent license is available.

Patent No. : USP6878666, 6864211, 6838413, 7015171, 7670712 Patent owner contact: Masaru OZAKI (JST) Tel:+81-3-5214-8486 e-mail: license@jst.go.jp

 Using photocatalysts to extend the absorption edge to longer wavelengths



Measurement of Water Isotopomers and its Applications

1. Water Isotopomers (WI)

Isotopomers of water molecule

H2O O			
Isotopomer ratio	Rel. abundance	Conventional technique	Expressio n
HD ¹⁶ O/H ₂ ¹⁶ O	0.03%	Reduction to H_2 H_2 equilibration with Pt catalyst Laser spectroscopy	D*1
H ₂ ¹⁸ O/H ₂ ¹⁶ O	0.20%	CO ₂ equilibration Laser spectroscopy	¹⁸ O
H ₂ ¹⁷ O/H ₂ ¹⁶ O	0.04%	Fluorination with BrF_5 (CoF ₃)	¹⁷ O

*1: D (‰) = (D/H)_{sample} / (D/H)_{VSMOW} - 1 VSMOW: Vienna Standard Mean Ocean Water provided by IAEA and NIST/USA

Prof. Naohiro YOSHIDA (Tokyo Institute of Technology)

- Analysis of WI is applicable to;
 - global environments
- traceability of foods
- medical cares -
- criminal investigations



Global mapping of isotope ratio (¹⁸O) in precipitation

2. Rapid and Precise WI Analysis by Water Electrolysis Device (WED)



Comparison with other techniques

	Equilibration	Fluorination (for O) Reduction (for H)	Laser Spectroscopy	WED
Advantage	Longest history Commercially available	Micro-liter sample Commercially available (reduction)	Micro-liter sample Fastest analysis	Fast analysis Micro-liter sample
Disadvantage	Slowest analysis Difficult for micro-liter	Chemical hazardous Difficult to control	Worst precision	
¹⁷ O analysis	Possible but difficult	OK (by fluorination)	Impossible	OK

3. Applications of WI Analysis-Environment, Food and Human Diagnosis

Historical change of global temperature reconstructed from Antarctic Ice Core.



Watanabe, Yoshida, et al. (Nature, 2003)

Metabolic energy measured by doubly labeled water (DLW) method



Geographic origin (cultivation regions) identified using 180 of wine water.



4. Patent status & Patent owner contact

Patent license is available.

Patent No. : WO00/49640. WO00/58712 Apply country : JP,US, EU Patent owner : JST, Tokyo Institute of Technology

Contact: O.KANZAKI (JST) Tel:+81-3-5214-8486 e-mail: license@jst.go.jp

Dr. Kazuhiro CHIBA (Tokyo University of Agriculture and Technology)

1. Introduction

Basic Technology Chemical Synthesis in biphasic miscible organic solution



biphasic miscible organic solution

Example of Application Product Separation in biphasic immiscible solvents



2. Application for peptide synthesis







Synthesis of a TNF-a Antagonist

Synthesis of Somatostatin



Up to equimolar reactions

Bridge formation



Varied modifications





3. PeptuneTM (commercially available product) approach

Introducing a new bridge chemistry with linker function to introduce steric constraint



Functional moiety can be appended on bridgehead position in addition N, C terminal position

Peptune[™] provides new peptide scaffolds with artificial bridge which is;

1. introducing other functional moiety into peptide's backbone as well as controlling structural constraint of peptides

2. as a similar approach to medicinal chemistry

3. with a unique liquid phase synthesis method

4. applicable to peptide therapeutics, delivery motives, and diagnostics

4. Patent status & Patent owner contact

Patent license is available. Patent No. : 3538672(JP) and others Applied in : JP,US,EP,CN Patent owner contact : Osamu KANZAKI Tel: +81-3-5214-8486 e-mail: license@jst.go.jp Peptune patent filed in worldwide by JITSUBO Co.Ltd., a Japanese licensee of JST for the basic patent and also available for licensing.

Ultrasonic Elasticity Imaging of Arterial Wall for Tissue Characterization

[Summary]

Diagnosis of vulnerability of atheroma is important for prevention of cardiovascular and cerebrovascular events. We have developed a method for measurement of the regional elasticity of the arterial wall with transcutaneous ultrasound. This method has potential for noninvasive tissue characterization of artery wall.

[Phased Tracking Method]

for measuring small change in thickness (strain) of artery wall caused by heartbeat



[Elasticity Imaging]

by measuring spatial distribution of changes in thickness (strain) and systolic/diastolic blood pressure measured with cuff at brachial artery

Prof. Hiroshi KANAI (Tohoku University)



Transcutaneously Measured Carotid Elasticity Images



[Elasticity Library 1] fibrous tissue=mixture of collagen and smooth muscle for detecting fibrous tissue and lipids

Elasticity distributions of fibrous tissue and lipids were determined by referring to pathological images. 1.3 2 - **0**.5 3.00 lipids smooth muscle [determined elasticity distributions] [Elasticity Library 2] for determining collagen content in fibrous tissue

[collagen vs. smooth muscle]

and smooth muscle.

Fibrous tissue almost consist of fibrous tissue

Elasticity value and collagen content in corresponding region were compared.



[collagen content vs. elasticity] regression line: E=0.013·CC+1.5 [MPa] (E: elasticity, CC: collagen content)

plots: spatial mean in 600 × 600 µm vertical bars: standard deviation

3 mm 3 mm nus tis li ti d n of fibrous cap 3 mm collagen

[Transcutaneous Tissue Characterization]

[Patent Status & Patent Owner Contact] patent No.: WO2003/015635 patent owner contact: Yoshihiro MURAI (JST) Tel:+81-3-5214-8486 E-mail: license@jst.go.jp

[References]

- 1) H. Kanai, et al.: IEEE Trans. UFFC, 1996, 1997, 1999.
- H. Kanai, et al.: Circulation, 108, 3018-3021, 2003.
 J. Inagaki, et al.: Jpn. J. Appl. Phys., 2005, 2006.
 K. Tsuzuki, et al.: Ultrasound Med. Biol., 2008.
- 5) K. Tsuzuki, et al.: Jpn. J. Appl. Phys., 2008
- 6) H. Hasegawa, et al: IEEE Trans. UFFC, 2004, 2006, 2008.

Atomic Switch Arrays for Memory and Logic Circuits

Dr. Tsuyoshi HASEGAWA (National Institute for Material Science)

1. Nanoionic Devices

Nonvoaltile switches for memory and logic operations in the beyond 16nm generation.



Filament formation and annihilation



ReRAM : Anion-based resistive switch Atomic Switch: Cation-based resistive switch



Hybrid CMOS/Nanoelectronic circuit

2. Cation-based resistive switch: Atomic switches

Two types of atomic switches.

Gap-type atomic switch



Gapless-type atomic switch



Specifications

Retention time: 10 years Scalability: 10 nm Switching time: 1 ns. Cyclic endurance: 10⁵ times

Materials



Active Electrode: Cu, Ag Ionic conductor: Ag₂S, Cu₂S, Ta₂O₅, HfO₂, SiO₂,

3. Application of atomic switches

Logic gates





• Multi-state memories, adder circuit, etc.



4. Patent status & Patent owner contact

Patent license is available.

Patent No. : WO2002-037572 Apply country : JP,US,TW,EP,KR Patent owner contact: Hisahiro Moriuchi (JST) Tel:+81-3-5214-8486 e-mail: license@jst.go.jp

New Pump-probe Technique providing a Wide Range Time-scale and Nanoscale Measurement

Prof. Hidemi SHIGEKAWA (University of Tsukuba)

1. New pump-probe technique

Delay Time Modulation Femtosecond Time-resolved Scanning Probe Microscope



(1)Conventional optical intensity modulation causes the tunnelling current change by the thermal effect.

(2)Delay time modulation using pulse pickers gives: wide time rage measurement (femtosecond ~ microsecond) overcome of the thermal effect

temporal resolution deternined by pulse width and spatial resolution determined by STM

3. Examples by nanoscale pump-probe

Real space imaging of transient carrier dynamics in the nanostructures with a wide variety of lifetimes

3-1. Carrier lifetimes measured by STM

 $\cdot\, \mbox{Time-dependent}$ STM signals can be obtained for various materials

• Decay times of photoexcited carriers are consistent with the lifetimes measured by conventional optical pump-probe method.



2. new key method

2-1. new delay-time modulation

Delay time is controlled in a digital form using pulse pickers.



2-2. New Lock-in measurement

Delay time t_d is modulated between t_{d1} (measurement point) and a large value of t_{d2} . The signal $S(t_d)$ is measured by lock-in detection technique.

The output of the lock-in amplifier directly provides $S(t_{d1})$.



3-2. Imaging nanoscale carrier dynamics

Observation of diffusion and drift on carrier recombination processes in an inner potential of GaAs PIN structure: Decay of photocarrier density is apparently accelerated in the I-region.

a: measuring method. b: band structure.

c: a series of time-dependent carrier density images.

d: mapping of decay time obtained from the full series of the time-dependent STM images.

e: decay time d (cross section along the line in d.)



6. Patent status & Patent owner contact

Patent license is available.

Patent No. : WO 2008/066090, WO 2003/046519 Apply country : JP,US,EP,CA,CN,KR JP,US,EP Patent owner contact: Hisahiro Moriuchi (JST) Tel:+81-3-5214-8486 e-mail: license@jst.go.jp

Electronic State Calculation Method, Computer Program, by Fluctuation-Referenced Multi-Reference DFT

Prof. Dr. Koichi KUSAKABE (Osaka University)

1. What is MR-DFT?

Our MR-DFT realizes

- Inclusion of quantum fluctuation,
- Systematic improvement of LDA, etc.

	Single-referenced Kohn- Sham DFT-LDA	Multi-referenced extended KS DFT
Reference	W. Kohn and L.J. Sham, Phys. Rev. 140 (1965) A1133.	K. Kusakabe, JPSJ 70 (2001) 2038; <i>ibid</i> 78 (2009) 114716.
Formal self-consistency in calculation scheme		
Ab-initio determination of model functionals	Extrapolation	
Variational principle for model functionals	×	

3. New technique developed!

Production of a model sequence in the model space (a Banach space).

A schematic example

Exact solution of electron system with Coulombic correlation Quantum fluc. in full bands •Multi-band correlation

Convergence area

Quantum fluc. around E_F •CDW, SDW •Super. or MI tr. Quantum fluc. in many bands •Multi-band ex-Hubbard

A quantum phase transition

- DFT LDA, GGA
- •Charge dens.
- •Spin density
- Band structure

Quantum fluc. In an isolated band •Single band Hubbard model

Convergence w.r.t. charge distance a converged model in the model space.

Theorems: J. Phys. Math. Theor. 44 (2011) 135305. K. K. & I. Maruyama: Japan patent submitted : JP 2010-183375.

5. Patent status & Patent owner contact

Patent license is available.

Patent No. : WO2010-023943 Apply country : JP, US(allowed) Patent owner contact: Hisahiro Moriuchi (JST) Tel:+81-3-5214-8486 e-mail: h2moric@jst.go.jp

2. How MR-DFT is given?

- Based on an energy functional, $F_{X_i}[n] = \min_{\Psi \to n(\mathbf{r})} \langle \Psi | \hat{T} + \sum_{n} \Xi_n^{(i)} (\hat{Y}_n^{(i)} - \langle \hat{Y}_n^{(i)} \rangle, \hat{Z}_n^{(i)} - \langle \hat{Z}_n^{(i)} \rangle) \Psi \rangle.$
 - JPSJ 70 (2001) 2038.
- Variational principle is given.
 - JPSJ 78 (2009) 114716.
 1st principles extended Hubbard model
 Band calc. with corr. in relevant bands.
 Self-consistent solution

4. Applications

Layered superconductors with high T_{c}



$$F_{n_{1},\mathbf{k}_{1},n_{2},\mathbf{k}_{2}} = \left\langle \phi_{n_{1},\mathbf{k}_{1}}\phi_{n_{2},\mathbf{k}_{2}} \left| \hat{V}_{ee} \right| \varphi_{n_{c},(\mathbf{k}_{c},l=0)} \varphi_{n_{c},(-\mathbf{k}_{c},l=0)} \right\rangle$$

$$J' = -\sum_{n_1 \neq n_c, \mathbf{k}_1} \frac{\left|F_{n_1, \mathbf{k}_1, n_1, -\mathbf{k}_1}\right|^2}{\left|\mathcal{E}_{n_1, \mathbf{k}_1, n_1, -\mathbf{k}_1} - \mathcal{E}_{n_c, (\mathbf{k}_c, k_z)}\right|}$$

Convergence certified by our patent.

New 3-way catalytic reaction

NO_x reduction on LaO/LaFeO₃. (H. Kizaki & K.K., Surf. Sci. in press.)

The ER scheme Pd nano-particle CO+O[•] $CO_2 NO_y, N_2 NO_x$ Pd oxide film V o[•] V V V



K.K. & H.Kizaki: Japan patent submitted : JP 2009-204665.

A solution for the element science & technology.

Design of graphene devices



The array of Quantum dots in 200Tbit/cm² is



A localized orbital



: Periodic Anderson model by our patent.

= a quantum dot

Lignin-based Solar Cell

1. Utilization of Forest Resources

Lignin has never been utilized sufficiently as industrial material.



Pulp & Paper

2. Phase-separation Method

Easy Separation of Carbohydrates and Lignin Derivatives



3. Lignin-based Solar Cell Structure



12

10

8

6

4

2

0

0

Photocurrent density / mAcm⁻²

Proposed mechanism

I Ps

e⁻ S+/S*

Accepto

r I₃

s*/sº

Dono

Electrolyte

e



4. Patent status & Patent owner contact

Patent license is available.

 $V_{oc} = 0.51 V$

= 3.6 %

ff = 0.59

I_{sc} = 10.23 mAcm⁻² W_{max} = 3.1 mWcm⁻²

Under visible and Infrared light (85.0 mWcm⁻², > 400 nm)

> Patent No. : WO2004/070868, JP3934068 Apply country : JP,US,EP,KR,CN Tel:+81-3-5214-8486 Patent owner contact: Masaru OZAKI (JST)

0.1 0.2 0.3 0.4 0.5 0.6 Photovoltage / V

e-mail: license@jst.go.jp

Prof. Masamitsu FUNAOKA (Mie University)



Japan Science and Technology Agency Center for Intellectual Property Strategies 5-3, Yonbancho, Chiyoda-ku, Tokyo, 102-8666 JAPAN Phone: +81-3-5214-8486 Fax: +81-3-5214-8487 E-mail: license@jst.go.jp URL: http://www.jst.go.jp/tt/EN/univip/cips/licensing.html