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Synthesis, Ionic Conductivity, and Thermal Properties of Proton Conducting Polymer Electrolyte for High Temperature Fuel Cell, Takahito ITOH, Yohei HAMAGUCHI, Takahiro UNO, Masataka KUBO, Yuichi AIHARA*, Atsuo SONAI* : Solid State Ionics 177, pp. 185-189, 2006

Hyperbranched polymer (poly-1a) with sulfonic acid groups at the end of chains was successfully synthesized. Interpenetration reaction of poly-1a with a hyperbranched polymer with acryloyl groups at the end of chains (poly-1b) as a cross-linker afforded a tough electrolyte membrane. The poly-1a and the resulting electrolyte membrane showed the ionic conductivities of 7×10^{-4} and 8×10^{-5} S/cm, respectively, at 150 °C under dry condition. The ionic conductivities of the poly-1a and the electrolyte membrane exhibited the VTF type temperature dependence. And also, both poly-1a and the resulting electrolyte membrane were thermally stable up to 200 °C.

Solid Polymer Electrolytes Based On Comblike Polymers, Takahito ITOH, Yukihiro MITSUDA, Katsumi NAKASAKA, Takahiro UNO, Masataka KUBO, Osamu YAMAMOTO* : Journal of Power Source 163, pp. 252-257, 2006

New comblike polymers such as a homopolymer (poly-4) of 3,5-bis[poly(ethylene glycol) methyl ether (350, $n=7.2$)]styrene (4) and an alternating copolymer (poly-4/TCNQ) of 4 with 7,7,8,8-tetracyanoquinodimethane (TCNQ) were prepared as a plasticizer for the poly(ethylene oxide) (PEO)-LiN(CF₃SO₂)₂ electrolyte, and the ionic conductivities, thermal property, electrochemical and thermal stabilities, and mechanical property for the comblike-based polymer electrolytes, composed of the comblike polymers, poly(ethylene oxide) (PEO), and LiN(CF₃SO₂)₂, were investigated. The polymer electrolytes containing an alternating copolymer poly-4/TCNQ showed the higher ionic conductivity, better thermal stability and better mechanical stability than that containing a homopolymer poly-4, due to the presence of an aromatic ring and a polar cyano group of the TCNQ unit.

Solid Polymer Electrolytes Based on Poly(1,3-diacetyl-4-imidazolin-2-one), Hiroyuki MITSUDA, Takahiro UNO, Masataka KUBO, Takahito ITOH : Polymer Bulletin 57, pp. 313-319, 2006

Solid polymer electrolytes composed of a homopolymer (poly(AcIM)) of 1,3-diacetyl-1,4-imidazolin-2-one (AcIM) and lithium bis(trifluoromethanesulfonimide) (LiTFSI) or of copolymers (poly(AcIM/VC)) of AcIM with vinylene carbonate (VC) and LiTFSI were prepared and their ionic conductivities and thermal properties were investigated. For the polymer electrolyte of the poly(AcIM) with LiTFSI, the highest ionic conductivity was found at the [Li]/[O] ratio of 1/3 with the values of 8.5×10^{-5} S/cm at 80 °C and 1.7×10^{-6} S/cm at 30 °C, respectively. In the polymer electrolyte of poly(AcIM/VC) with LiTFSI at the [Li]/[O] ratio of 1/3, the ionic conductivity increased with increasing VC unit content in the copolymers, and the highest ionic conductivity was found at the AcIM/VC ratio of 39/61 (mol%) with the values of 7.0×10^{-4} S/cm at 80 °C and 6.7×10^{-5} S/cm at 30 °C, respectively. This copolymer electrolyte showed a linear relationship between the ionic conductivity and the reciprocal of the temperature, indicative of the system decoupled from the segmental motion of the polymer.

Synergistic effect of red phosphorus, novolac and melamine ternary combination on flame retardancy of

poly(oxymethylene), Hatsuhiko HARASHINA, Yoshihisa TAJIMA*, Takahito ITOH : Polymer Degradation and Stability 91, pp. 1996-2002, 2006

New flame retardant system for poly(oxymethylene) (POM) has been studied. The combination of red phosphorus with novolac and melamine was found to act as an effective flame retardant of POM. The base POM exhibited very low limiting oxygen index (LOI) value of 15.3, while the flame retarded POM gave remarkably high LOI value of 37.5 and UL94 V-1 ranking without dripping at 0.8mm thickness. The results of cone calorimetry, thermogravimetry and FTIR analysis suggested that the flame retarding mechanism is the intumescent char formation in the condensed phase. Novolac having a phenolic hydroxyl group is miscible with POM, and in the flaming process, red phosphorus yields phosphine and its acidic product such as phosphoric acid due to hydrolysis and oxidation reactions. In addition, all of novolac, melamine and phosphine are able to readily react with formaldehyde generating from POM during burning to give the reinforced and cross-linked char network through the polyaddition and polycondensation reactions. Therefore, the red phosphorus/novolac/melamine ternary combination system could synergistically promote the high flame retardancy of POM without the flaming drips.

Topochemical Reaction of 7-Bromoethoxycarbonyl-7-cyano-1,4-benzoquinone Methide in the Solid State, Takahito ITOH, Kyoko TACHINO, Takahiro UNO, Masataka KUBO, Norimitsu TOHNAI*, Mikiji MIYATA* : Chemistry Letters 35(8), pp. 918-919, 2006

Topochemically controlled [2 + 2] photocycloaddition took place at the quinonid double bond of the 7-bromoethoxycarbonyl-7-cyano-1,4-benzoquinone methide (1) to afford its cyclobutane dimer.

Synthesis, Ionic Conductivity, and Thermal Properties of Hyperbranched Polymer with Phosphonic Acid Groups at the Chain Ends for High Temperature Fuel Cell, Takahito ITOH, Yohei HAMAGUCHI, Keita HIRAI, Takahiro UNO, Masataka KUBO, Yuichi AIHARA*, Atsuo SONAI* : ECS Transactions (Proton Exchange Membrane Fuel Cells 6) 3, pp. 113-121, 2006

Two different molecular weight hyperbranched polymers (HBP-PA(L) and HBP-PA(H)) with phosphonic acid groups at the chain ends were successfully synthesized. The ionic conductivities of the low molecular weight HBP-PA(L) and the high molecular weight HBP-PA(H) were found to be 1.3×10^{-4} and 6.4×10^{-5} S/cm, respectively, at 135 °C under dry condition, and showed the VTF type temperature dependence. And also, both polymers were thermally stable up to 300 °C, and they had suitable thermal stability as an electrolyte in the polymer electrolyte fuel cell operating under dry condition.

Emission from Silica Hybrid Containing RGB Fluorescent Conjugated Polymers, Yuya SUGIURA, Masashi SHOYAMA*, Koji INOUE*, Takahiro UNO, Takahito ITOH, Masataka KUBO : Polymer Bulletin 57, pp. 865-871, 2006

Red, green and blue fluorescent poly(arylene vinylene)s were prepared by Wittig reaction. Polycondensation of tetraethoxysilane (TEOS) was carried out in the presence of a mixed solution of these polymers to give a silica hybrid in which RGB fluorescent polymers were immobilized without phase separation. White light emission was observed from the ternary polymer blend/silica hybrid.

Nonbonding cross-linking agent, Masataka KUBO : Hyomen 44, pp. 337-344, 2006

Development of hybrid EL film by sol-gel method, Masataka KUBO, Masashi SHOYAMA* : Monthly DISPLAY 12, pp. 43-47, 2006

Titanium Tetraiodide Mediated Reductive Opening of Aziridines, Leading to the Aldol and Mannich-Type Reactions, Makoto SHIMIZU, Hiroshi KUROKAWA, Shuji NISHIURA, Iwao HACHIYA: Heterocycles, 70 (1), pp. 57-64, 2006

3,4,5,6-Tetrasubstituted-2-pyridone Synthesis via Nucleophilic Addition of Active Methine Compounds to Dialkynyl Imines Directed to the Synthesis of (-)-A58365A, Iwao HACHIYA, Shiho FUKUSHIMA, Makoto SHIMIZU: Heterocycles, 69 (1), pp. 43-48, 2006

Ring Expansion Reaction of Cyclic α -Keto Esters or α -Cyano Ketones via Conjugate Addition to Alkynyl Imines: The Synthesis of Functionalized Medium-Sized Carbocycles, Iwao HACHIYA, Wataru MAEHARA, Yasushi YAMADA, Toru KAMIKI, Makoto SHIMIZU: Synlett, (19), pp. 3271-3274, 2006

Efficient Asymmetric Synthesis of Novel Gastrin Receptor Antagonist AG-041R via Highly Stereoselective Alkylation of Oxindole Enolate, Takashi EMURA, Toru ESAKA*, Kazutaka TACHIBANA*, Makoto SHIMIZU: J. Org. Chem., 71 (22), pp. 8559-8564, 2006

Unexpected and Intriguing Reactivity of α -Imino Esters and Iminium Salts, Makoto SHIMIZU: Pure Appl.Chem., 78 (10), pp. 1867-1876, 2006

Efficient Pyrrole Synthesis Using Double Nucleophilic Addition to α,β -Unsaturated Imines with Plural Nucleophiles, Makoto SHIMIZU, Atsushi TAKAHASHI, Shiho KAWAI: Org. Lett., 8 (16), pp. 3585-3587, 2006

Remarkable Effects of Additives to Facilitate Aza-Mannich Type Reaction: A Rapid Access to α -Amino Ketone *O*-Alkyl Oximes, Makoto SHIMIZU, Mitsue TANAKA, Tomohiro ITOH, Iwao HACHIYA: Synlett, (11), pp. 1687-1690, 2006

New Synthetic Reactions Using Conjugate Addition Reactions of Active Methine Compounds to Alkynyl Imines and Ketones [in Japanese], Iwao HACHIYA, Makoto SHIMIZU, J. Synth. Org. Chem., Jpn., 64 (3), pp. 251-262, 2006

Synthesis of Bicyclic Compounds Containing a 2-Pyridone Structure by Addition of Malonic Esters to

Alkynylpyridines, Pyrimidine, and Thiazoles, Iwao HACHIYA, Masaki ATARASHI, Makoto SHIMIZU: *Heterocycles*, 67 (2), pp. 523-528, 2006

Rigid Molecular Tripod with an Adamantane Framework and Thiol Legs. Synthesis and Observation of an Ordered Monolayer on Au(111), Toshikazu KITAGAWA, Yuichi IDOMOTO*, Hiroaki MATSUBARA*, Daisuke HOBARA*, Takashi KAKIUCHI*, Takao OKAZAKI*, Koichi KOMATSU*: *J. Org. Chem.*, 71(4), pp. 1362-1369, 2006

Synthesis of Disubstituted Homodiamantanes by Acylative Ring Expansion Using Benzoyl Trifluoromethanesulfonate, Takao OKAZAKI*, Shusaku MANDAI*, Toshikazu KITAGAWA, and Ken'ichi TAKEUCHI*: *Sci. Tech. Adv. Mater.*, 7(6), pp. 531-535, 2006

Triplet Diphenylcarbenes Protected by Trifluoromethyl and Bromine Groups. A Triplet Carbene Surviving a Day in Solution at Room Temperature, Tetsuji ITOH, Yoshimaru NAKATA, Katsuyuki HIRAI*, and Hideo TOMIOKA*: *J. Am. Chem. Soc.*, 128(3), pp. 957-967, 2006

A Dendrimer Approach to High-Spin Polycarbenes. Conversion of Connectivity from Disjoint to Non-Disjoint by Perturbation of Nonbonding Molecular Orbital Coefficients, Katsuyuki HIRAI*, Eiko KAMIYA, Tetsuji ITOH, and Hideo TOMIOKA*: *Org. Lett.*, 8(9), pp. 1847-1850, 2006

Theoretical Study of Electronic Structures of [Peroxoporphinato]manganate $[\text{Mn}(\text{P})(\text{O}_2)]^-$ Anion, Yasunori YOSHIOKA, Hideaki SANO, Masaki MITANI: *Bull. Chem. Soc. Jpn.*, 79 (8), pp. 1201–1210, 2006

Geometries and electronic structures of the quintet and septet states of the $[\text{Mn}(\text{P})(\text{O}_2)]^-$ (P: porphinato) anion were theoretically investigated. Four local minimum geometries with two side-on additions of O_2 to MnP, **1** ($^5\text{B}_2$) and **3** ($^7\text{A}_2$), and two end-on additions of O_2 , **2** ($^5\text{A}''$) and **4** ($^5\text{A}'$), were found. One of the side-on forms, **1**, corresponds to that observed by X-ray crystallographic study. **3** is a septet state with higher spin than the quintet states of **1**, **2**, and **4**. Each of the two end-on forms has the corresponding transition state with the side-on geometry. Energy differences among **1**, **2**, and **3** are less than 1 kcal mol^{-1} . The electronic structures of four local minimum states were essentially different. **1** has an electronic structure presented as $[\text{Mn}^{\text{III}}(\text{O}_2^{2-})]^-$. **2** has antiferromagnetically coupled diradical character presented by the formal chemical formula of $[\text{Mn}^{\text{II}}(\text{O}_2^{\bullet-})]^-$. **3** has ferromagnetically coupled diradical character. **4** is presented by $[\text{Mn}^{\text{II}}(\text{O}_2^-)]^-$.

Electronic Structures of Heme(Fe)–Dioxygen Complex as an Intermediate Model of Dioxygen Reduction in Cytochrome *c* Oxidase, Yasunori YOSHIOKA, Masaki MITANI, Hiroyuki SATOH: *Internet Electron. J. Mol. Des.*, 5 (8), pp. 447–459, 2006

We have previously proposed the O_2 reduction mechanism that the protons transfer from the K-channel to the active site of CcO. The second proton transfer to the hydroperoxy intermediate FeOOH did not lead the OO bond cleavage. It has been recently reported that the addition of the proton induces the OO bond cleavage to yield the productive H_2O molecule and the oxo intermediate $\text{Fe}=\text{O}$, being inconsistent with our results. We have started this

study to confirm whether the OO bond cleavage occurs or not upon the proton addition. We concentrated our study to the changes of the electronic structures of the heme *a3* part throughout the sequential additions of the protons and an electron during the process of the O₂ reduction. We employed a model that is composed of porphyrin without any substituents, Fe, and an imidazole as His376. We added sequentially protons and an electron to the heme(Fe)–dioxygen complex. The geometrical parameters were fully optimized without any constraints. The unrestricted hybrid exchange–correlation functional B3LYP method was used. The Wachters double zeta basis set was employed for Fe atom. The 6–31G* basis set was used for C, N, and H atoms, and the 6–311+G* for O atom. All calculations were carried out using the program package Gaussian 98. The proton addition to FeOO (H2) to yield FeOOH (H3) causes the electron transfer from the porphyrin ring to FeOOH moiety, giving the porphyrin–radical cation. The additional proton to FeOOH (H4) leads to the OO bond cleavage, yielding the hydrogen bonded complex of an oxo heme (compound I) and a H₂O molecule. The bonding characters of FeOOH in H3 and H4 are identical, even though the electronic structures of the porphyrin rings in H3 and H4 are different. However, the proton addition to FeOOH (H3) does not lead to the OO bond cleavage. The protonated heme(Fe)–dioxygen complexes are effective models to investigate the reduction mechanism of a O₂ molecule in CcO.

A B3LYP Study of Proton Transfer Path within a Complex of Benzene Radical Cation and Water Cluster, Moriyuki SHIMIZU, Emi YAMASHITA, Masaki MITANI, Yasunori YOSHIOKA: *Chem. Phys. Lett.*, 432, pp. 22–26, 2006

We made a theoretical study of the proton transfer path from C₆H₆^{•+}(H₂O)₄ to C₆H₅[•](H₂O)₄H⁺ with a planar cyclic geometry of (H₂O)₄H⁺ by the hybrid density functional B3LYP method. The proton transfer proceeds in a three-step manner. In the first step, the proton in C₆H₆^{•+}(H₂O)₄ moves from the terminal H₂O molecule in the (H₂O)₄ cluster to yield a (H₂O)₃H⁺ cluster. In the last third step, one H₂O molecule leaves from C₆H₆(OH)[•] in C₆H₆(OH)[•](H₂O)₃H⁺ to yield a C₆H₅[•](H₂O)₄H⁺ complex through the H-abstraction by the OH radical. It is found that the proton transfer and redistribution from p to r of the radical electron proceed separately.

Highly Activated Vinyl Hydrogen in a Significantly Twisted Styrene, Hajime MORI*, Takafumi MATSUO*, Yasunori YOSHIOKA, Shigeo KATSUMURA*: *J. Org. Chem.*, 71 (24), pp. 9004–9012, 2006

The novel example of a vinylic hydrogen more reactive than a benzylic hydrogen was found by treatment of a twisted styrene derivative with a strong base followed by D₂O quenching. In this paper, the full details of the examples of the highly activated vinyl hydrogens in twisted styrene derivatives are described, with a discussion on the correlation between the reactivity of the vinyl hydrogens and the magnitude of the twist. The highly reactive vinyl hydrogens could be rationalized by considering the novel orbital interaction between the π^* orbital of the benzene ring and the σ orbital of the vinylic C–H bond in the twisted styrene derivatives.

Density Functional Study on Geometrical Features and Electronic Structures of Di- μ -oxo-Bridged [Mn₂O₂(H₂O)₈]^{q+} with Mn(II), Mn(III), and Mn(IV), Masaki MITANI, Yohei WAKAMATSU, Takeharu KATSURADA, Yasunori YOSHIOKA: *J. Phys. Chem. A*, 110 (51), pp. 13895–13914, 2006

We report the geometrical features and electronic structures of di- μ -oxo-bridged Mn–Mn binuclear complexes with H₂O ligands [Mn₂O₂(H₂O)₈]^{q+} in the iso- and mixed-valence oxidation states. All of the combinations among Mn(II), Mn(III), and Mn(IV) ions are considered the oxidation states of the Mn–Mn center, and the changes in molecular structure induced by the different electron configurations of Mn-based orbitals are investigated in relation to

the oxygen-evolving complex (OEC) of photosystem II. The stable geometries of complexes are determined by using the hybrid-type density functional theory for both of the highest- and lowest-spin couplings between Mn sites, and the lowest-spin-coupled states are energetically more favorable than the highest-spin-coupled states except in the case of the complexes with the Mn(II) ion. The coordination positions of H₂O ligands at the Mn(II) site tend to shift from the octahedral positions in contrast to those at the Mn(III) and Mn(IV) sites. The shape of the Mn₂O₂ core and the distances between the Mn ions and the H₂O ligands vary depending on the electron occupations of the octahedral eg orbitals on the Mn site with an antibonding nature for the Mn–ligand interactions, indicating the trend as Mn(II)–O > Mn(III)–O and Mn(IV)–O, O–Mn(II)–O > O–Mn(III)–O > O–Mn(IV)–O among the iso-valence Mn₂O₂ cores, and O–Mn(lower)–O < O–Mn(higher)–O within the mixed-valence Mn₂O₂ core, and as Mn(II)–OH₂ and Mn(III)–OH₂ > Mn(IV)–OH₂ for the axial H₂O ligand. The optimized geometries of model complexes are compared with the X-ray structure of the OEC, and it is suggested that the cubanelike Mn cluster of the active site may not contain a Mn(II) ion. The effective exchange integrals are estimated by applying the approximate spin projection to clarify the magnetic coupling between Mn sites, and the superexchange pathways through the di-oxo bridge are examined on the basis of the singly occupied magnetic orbitals derived from the singlet-coupled natural orbitals in the broken-symmetry state. The comparisons of the calculated results between [Mn₂O₂(H₂O)₈]⁹⁺ in this study and [Mn₂O₂(NH₃)₈]⁹⁺ reported by McGrady et al. suggest that the symmetric pathways are dominant to the exchange coupling constant, and the crossed pathway would be less important for the former than it would for the latter in the Mn(II)–Mn(III), Mn(IV)–Mn(IV), and Mn(III)–Mn(IV) oxidation states.

Synthesis, structure, and electrochemical properties of epitaxial perovskite La_{0.8}Sr_{0.2}CoO₃ film on YSZ substrate, Daisuke Mori*, Hideaki Oka*, Yoshitaka Suzuki*, Noriyuki Sonoyama*, Atsuo Yamada*, Ryoji Kanno*, Yoshiaki Sumiya, Nobuyuki Imanishi and Yasuo Takeda : Solid State Ionics 177, pp. 535-540, 2006

Epitaxial films of the perovskite, La_{0.8}Sr_{0.2}CoO₃ (LSC), for SOFCs cathode were deposited on yttria-stabilized zirconia (YSZ) single crystals by pulsed laser deposition method. The films were characterized by thin-film X-ray diffraction measurement, atomic force microscopy (AFM), transmission electron microscope (TEM), and ac impedance spectroscopy. The film orientations depend on the substrate planes. The LSC films on the YSZ (100) and (111) substrates showed the (110) orientation with different twin structures, while those on the YSZ (110) had (100) and (112) orientations. Surface morphology of the films also depends on the substrate orientations. These films showed different electrode properties depending on the orientations. The relationships between the properties, the film orientations, surface morphology, and lattice misfit are discussed.

An anomalous thermal expansion in the perovskite system, Gd_{1-x}Sr_xMnO₃ (0 ≤ x ≤ 0.3), A. Hirano, F. Hirano, T. Matsumura, N. Imanishi and Y. Takeda : Solid State Ionics 177, pp. 749-755, 2006

The thermal expansion behavior of sintered samples of Gd_{1-x}Sr_xMnO₃ (X=0.0–0.4) was studied. The sintered bodies in this system showed negative thermal expansion over a wide temperature range. The detailed crystal structure refinements with respect to temperature showed that the volume of the orthorhombic perovskite lattice monotonically increased with temperature, however, in addition to this, the release of distortion from the Jahn-Teller effect of Mn³⁺ ion occurred over a wide temperature range, which brought the negative expansion of the *a*-axis, although the *b*- and *c*-axes increased with temperature. The anomalous thermal expansion is explained by the sum of the effects of the shrinkage of the *a*-axis and absorption of the *b*- and *c*-axes' expansion by the pores in the sintered body.

Preparation and electrochemical properties of a $\text{Li}_2\text{CuO}_2\text{--Li}_2\text{NiO}_2$ solid solution as a lithium-intercalation electrode, N. Imanishi, K. Shizuka*, T. Ikenishi, T. Matsumura, A. Hirano and Y. Takeda : *Solid State Ionics* 177, pp. 1341-1346, 2006

Solid solution materials of Li_2CuO_2 and Li_2NiO_2 were studied with respect to their electrochemical performance and crystal structure. The $\text{Li}_2\text{CuO}_2\text{--Li}_2\text{NiO}_2$ system shows a solid solution over the whole composition range with the orthorhombic structure. Pure Li_2CuO_2 has a reversible capacity of only 100 mA h/g, and the capacity of $\text{Li}_2\text{Cu}_{1-x}\text{Ni}_x\text{O}_2$ increased with increasing the content of Ni. The maximum capacity of 250 mA h/g is obtained for $\text{Li}_2\text{Cu}_{0.5}\text{Ni}_{0.5}\text{O}_2$, and it exhibits a good reversibility for charge and discharge cycles. The orthorhombic Li_2CuO_2 undergoes a phase change to the monoclinic LiCuO_2 during lithium deintercalation, while nickel-rich compositions show a new phase that is different from either the original orthorhombic or monoclinic structure.

Impedance study and TEM characterization of a PLD perovskite air electrode, Nobuyuki Imanishi, Yoshiaki Sumiya, Ken Yoshimura, Tadaaki Matsumura, Atsushi Hirano, Yasuo Takeda, Daisuke Mori* and Ryoji Kanno* : *Solid State Ionics* 177, pp. 2165-2173, 2006

TEM observation and electron diffraction analysis of a laser ablation perovskite film was carried out. The film was deposited on a single-crystal substrate and showed epitaxial growth normal to the substrate. The crystal orientation of the perovskite film varies depending on the kind of single-crystal substrate. The surface structure of the atomic arrangement was investigated based on an analysis of electron diffraction patterns. Its relation to the kinetics of the reduction of molecular oxygen is discussed.

Novel Composite Anodes Consisting of Lithium Transition-Metal Nitrides and Transition Metal Oxides for Rechargeable Li-Ion Batteries, Y. Liu, Y. Takeda, T. Matsumura, J. Yang*, N. Imanishi, A. Hirano, and O. Yamamoto* : *J. Electrochem. Soc.*, 153 (2) , pp. A437-A444 , 2006

Lithium transition-metal nitrides are promising anode candidates for Li-ion batteries. However, lithium must be extracted from the nitrides in an initial anodic oxidation, indicating these compounds cannot directly combine with the current cathodes to constitute cells. This deterrent can be overcome by introducing a certain amount of Co_3O_4 , which shows large capacities and relatively high oxidation/reduction potentials, into the electrodes containing the above nitrides. A thermodynamically spontaneous reaction between these two active hosts results in a delithiated state of lithium metal nitrides. Under cycling within 1.4–0 V vs Li/Li^+ , Co_3O_4 is relatively inert to lithium and the nitrides become electrochemically active. The composite electrodes show high first-cycle efficiency of 100%, large capacities of 500 mAh g^{-1} , and excellent cyclability. Furthermore, research revealed that the composite electrodes demonstrated high cycling stability operating with polyethylene oxide (PEO) electrolytes at the elevated temperature. The reaction heating of the composite electrode under high Li utilization with PEO electrolytes via differential scanning calorimetry measurement was found to be extremely low compared with those of the lithium metal and the Li-alloy-based systems, suggesting that the composite electrodes could be promising anode candidates for all-solid-state PEO Li-ion batteries in terms of capacity, first-cycle charge efficiency, and thermal reliance.

Structural Changes and Electrochemical Properties of Chemically oxidized Na_xFeO_2 , Tadaaki Matsumura, Nobuyuki Imanishi, Atsushi Hirano, Ryoji Kanno* and Yasuo Takeda : *Journal of the Japan Society of Powder and Powder Metallurgy* 53 (11) , pp. 860-864, 2006

Na_xFeO_2 was obtained by chemical oxidization method using NO_2BF_4 and Br_2 which shows the redox potential of ca. 5.1 V and ca. 4.1 V vs Li / Li^+ , respectively. The oxidized products showed different X-ray diffraction patterns depending on the oxidizing species. In case of NO_2BF_4 , as soaking time progressed, new phase increased with decreasing of NaFeO_2 as starting material. The oxidized Na_xFeO_2 was possible to be inserted the Li ion electrochemically, and resulted in the crystal structure similar to the layered LiFeO_2 synthesized by the Li-ion-exchange method from NaFeO_2 . Reversible discharge-charge reactions were progressed for $\text{Na}_x\text{FeO}_2 // \text{Li}$ cell, and ac. 150 – 200 mAh/g of initial capacities were achieved although the capacities decreased with cycle numbers.

Effect of Silicon on the Formation of Graphitic Polyhedra and Balloon-like Particles, Fumio KOKAI, Noriko TAKAKUWA, Akira KOSHIO, Kunimitsu TAKAHASHI*: Applied Physics A, 84, pp. 391-394, 2006

Antibacterial Activity of Fluorine Incorporated DLC Films, Masatou ISHIHARA*, Tomomi KOSAKA*, Takako NAKAMURA*, Kazuo TSUGAWA*, Masataka HASEGAWA*, Fumio KOKAI, Yoshinori KOGA*: Diamond & Related Materials, 15, pp. 1011-1014, 2006

Electrochemical Reduction of CO_2 to Methane at the Cu Electrode in Methanol with Sodium Supporting Salts and Its Comparison with Other Alkaline Salts, Satoshi KANECO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Energy Fuels, 20, pp. 409–414, 2006

Photoelectrochemical Reduction of Carbon Dioxide at p-Type Gallium Arsenide and p-Type Indium Phosphide Electrodes in Methanol, Satoshi KANECO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Chem. Eng. J., 116, pp. 227–231, 2006

Sequential Molecular Vapor Elution Analysis for the Separation and Determination of LiCl and NaCl in River Waters, Yasutoshi SHIROTA, Md. Nurul AMIN, Yoshifumi WATANABE, Satoshi KANECO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Anal. Chim. Acta, 560, pp. 159–163, 2006

Photoelectrocatalytic Reduction of CO_2 in LiOH/Methanol at Metal-modified p-InP Electrodes, Satoshi KANECO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Appl. Catal. B: Environ., 64, pp. 139–145, 2006

Electrochemical Reduction of Carbon Dioxide to Ethylene at A Copper Electrode in Methanol Using Potassium Hydroxide and Rubidium Hydroxide Supporting Electrolytes, Satoshi KANECO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Electrochim. Acta, 51, pp. 3316–3321, 2006

Electrochemical Reduction of High Pressure CO_2 at A Cu Electrode in Cold Methanol, Satoshi KANECO, Keiji IIBA, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Electrochim. Acta, 51, pp. 4880–4885, 2006

Electrochemical Reduction of CO₂ in Copper Particle-suspended Methanol, Satoshi KANEKO, Yosuke UENO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Chem. Eng. J., 119, pp. 107–112, 2006

Fabrication of Visible Light Response Praseodymium-doped TiO₂ Photocatalysts and Its Application to Dye-sensitized Solar Cells, Naomi NISHIKAWA, Satoshi KANEKO, Hideyuki KATSUMATA, Tohru SUZUKI Kiyohisa OHTA, Yasuo TAKEDA, Masaki MURAYAMA*, Eiji YAMAZAKI*, Noritsugu HASHIMOTO*, Kazuaki MASUYAMA, Masashi SHOYAMA*: Photo/Electrochem. Photobiol. Environ. Energy Fuel, 5, pp. 311–319, 2006

Effect of Side-chain Structure on the Solar Photocatalytic Degradation of Phthalate Acid Esters, Satoshi KANEKO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Photo/Electrochem. Photobiol. Environ. Energy Fuel, 5, pp. 347–359, 2006

Titanium Dioxide Mediated Photocatalytic Degradation of Dibutyl Phthalate in Aqueous Solution—Kinetics, Mineralization and Reaction Mechanism, Satoshi KANEKO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Chem. Eng. J., 125, pp. 59–66, 2006

Removal of Arsenic in Aqueous Solutions by Adsorption onto Waste Rice Husk, Md. Nurul AMIN, Satoshi KANEKO, Taichi KITAGAWA, Aleya BEGUM, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA: Ind. Eng. Chem. Res., 45, pp. 8105–8110, 2006

Degradation of Polychlorinated Dibenzo-*p*-dioxins in Aqueous Solution by Fe(II)/H₂O₂/UV System, Hideyuki KATSUMATA, Satoshi KANEKO, Tohru SUZUKI, Kiyohisa OHTA, Yoshihiro YOBIKO*: Chemosphere, 63, pp. 592–599, 2006

Photo-Fenton Degradation of Alachlor in the Presence of Citrate Solution, Hideyuki KATSUMATA, Satoshi KANEKO, Tohru SUZUKI, Kiyohisa OHTA, Yoshihiro YOBIKO*: J. Photochem. Photobiol. A: Chem., 180, pp. 38–45, 2006

Determination of Atrazine And Simazine in Water Samples by High-performance Liquid Chromatography After Preconcentration with Heat-treated Diatomaceous Earth, Hideyuki KATSUMATA, Satoshi KANEKO, Tohru SUZUKI, Kiyohisa OHTA: Anal. Chim. Acta, 577, pp. 214–219, 2006

Degradation of Carbofuran by Cu/L-ascorbic acid/H₂O₂ System, Farzana FERDOUSH, Hideyuki KATSUMATA, Satoshi KANEKO, Tohru SUZUKI, Kiyohisa OHTA, Yoshihiro YOBIKO*: Photo/Electrochem. Photobiol. Environ. Energy Fuel, 5, pp. 321–334, 2006

Degradation of Diazinon in Aqueous Solution by V(IV)/H₂O₂ System, Hideyuki KATSUMATA, Hideyasu NAKAO, Farzana FERDOUSH, Satoshi KANECO, Tohru SUZUKI, Kiyohisa OHTA, Yoshihiro YOBIKO*: *Photo/Electrochem. Photobiol. Environ. Energy Fuel*, 5, pp. 335–345, 2006

Membrane Fusion between a Giant Vesicle and Small Enveloped Particles: Possibilities for the Application to Construct Model Cells, Kanta TSUMOTO, Koki KAMIYA, Tetsuro YOSHIMURA: *Proceedings of the International Symposium on Micro-NanoMechatronics and Human Science, MHS 2005 Micro-Nano COE, IEEE*, pp. 7-12, 2006

Antigen-Based Immunofluorescence Analysis of B-Cell Targeting: Advanced Technology for the Generation of Novel Monoclonal Antibodies with High Efficiency and Selectivity, Masahiro TOMITA, Takatomi FUKUDA, Akira OZU, Keiichi KIMURA, Tian Yow TSONG*, Tetsuro YOSHIMURA: *Hybridoma*, 25(5), pp. 283-292, 2006

A New Technology for the Generation of Novel Monoclonal Antibodies Based on Short-Term Immunization, Masahiro TOMITA, Yoshiharu ASAOKA, Yasuhiko KATO, Shin OGATA*, Tian Yow TSONG*, Tetsuro YOSHIMURA: *Peptide Science 2005*, pp. 105-108, 2006

Controlled Self-Assembly of Amphiphilic Oligopeptides into Shape-Specific Nanoarchitectures, Tomoyuki KOGA*: Masahiro HIGUCHI, Takatoshi KINOSHITA*, Nobuyuki HIGASHI*: *Chem. Eur. J.*, 12 (5), pp.1360-1367, 2006

Polymer Adsorption Effects on Stabilities and Chemical Mechanical Polishing Properties of Ceria Particles, Norifumi SHIMONO, Naoyuki KOYAMA*, Masami KAWAGUCHI: *Jpn. J. Appl. Phys.*, 45 (5A), pp. 4196-4200, 2006

Buoyancy-driven Path Instabilities of Bubble Rising in Simple and Polymer Solutions of Hele-shaw Cell, Masami KAWAGUCHI, Sukehiro NIGA, Nobuaki GOU, Kazuo MIYAKE: *J. Phys. Soc. Jpn.*, 75 (12), pp.124401-1-124401-6, 2006

Ti³⁺-Free Multicomponent Titanophosphate Glasses as Ecologically Sustainable Optical Glasses, Tadanori HASHIMOTO, Hiroyuki NASU and Kanichi KAMIYA: *J. Am. Ceram. Soc.*, 89 (8), pp. 2521-2527, 2006

Tunable Localized-Surface-Plasmon-Resonance Characteristics of Independently Prepared Ag-TiO₂ Particles, Noritsugu HASHIMOTO, Tadanori HASHIMOTO, Hiroyuki NASU, Yoshitsugu YAMAMOTO and Seiji NIIJIMA: *e-J. Surf. Sci. Nanotech.*, 4 (7), pp. 566-569, 2006

Cycle Performance of Sol-Gel Optical Sensor Based on Localized Surface Plasmon Resonance of Silver Particles, Noritsugu HASHIMOTO, Tadanori HASHIMOTO, Taichi TERANISHI, Hiroyuki NASU and Kanichi KAMIYA:

Sens. Actuators B, 113 (1), pp. 382-388, 2006

Photocatalytic Degradation of Allergens in Water with Titanium Dioxide, Naomi NISHIKAWA, Satoshi KANECO, Hideyuki KATSUMATA, Tohru SUZUKI, Kiyohisa OHTA, Eiji YAMAZAKI, Kazuaki MASUYAMA, Tadanori HASHIMOTO and Kanichi KAMIYA: Fresen. Environ. Bull., 16 (3), pp. 310-314, 2006

Addition Effect of Phosphorus on Ni-Mo Catalysts in Hydrodenitrogenation, Weihua QIAN, Satoshi ABE, Akinobu NOJIMA, Kenji GUNJI, Atsushi ISHIHARA, Hiroyuki IKEDA: Prepr. Pap.-Am. Chem. Soc., Div. Petr. Chem. 51(2), pp.271, 2006

PVC Hydrocracking with Recovering of a Large Amount of H₂. Characterization of the Catalysts and the Products after Each Step of the Process, Thierry GIORNELLI, Franck DUMEIGNIL, Atsushi ISHIHARA: Energy Efficient Technologies I-ACS, Green Chem. Inst., pp. 63, 2006

Intercellular localization of occludins and ZO-1 as a solute transport barrier of the mesothelial monolayer, Kenichi KANEDA, Keiichi MIYAMOTO, Shinsuke NOMURA, Takashi HORIUCHI: J. Artif. Organs., 9(4), pp.241-50, 2006

Development of a new method for endovascular aortic repair: combination therapy of cell transplantation and stent grafts with a drug delivery system, Masaki KAJIMOTO, Takatsugu SHIMONO, Kouji HIRANO, Youichi MIYAKE, Yashuhiro SAWADA, Noriyuki KATO, Hitoshi HIRATA, Kyoko IMANAKA-YOSHIDA, Masakatsu NISHIKAWA, Toshimichi YOSHIDA, Hideto SHIMPO, Takashi HORIUCHI, Keiichi MIYAMOTO: CIRCULATION 114, pp.1378-83, 2006

Evaluation of Compliance and Stiffness of Decellularized Tissues as Scaffolds for Tissue-Engineered Small Caliber Vascular Grafts Using Intravascular Ultrasound, Yousuke MURASE*, Yuji NARITA*, Hideaki KAGAMI*, Keiichi MIYAMOTO, Yuichi UEDA*, Minoru UEDA*, Toyooki MUROHARA*: ASAIO, 52, pp.450-455, 2006

An image analysis algorithm for kinematics and morphology measurement of cells for the evaluation of tissue construction, Tomoko GESSEI, Chie OTSUKA, Masatoshi BANNO, Keiichi MIYAMOTO, Yuji OHTA, Takashi HORIUCHI: IFMBE Proceedings, 14:2006