Molecular informatics: Preface to the special issue on the 21st century COE program of Kyushu University

This special issue of Science and Technology of Advanced Materials (STAM) presents the highlights of the research activities of Grants-in-Aid for the 21st Century COE Program “Functional Innovation of Molecular Informatics” of Kyushu University.

The development of novel molecules and materials via chemical science and technology is essential for innovation of materials research in chemistry. Novel molecules and their precisely controlled assembly would greatly promote the innovation of science and technology as a basic element of their functional properties. The Department of Applied Chemistry and other related groups at Kyushu University have already accomplished excellent research in the chemistry and molecular assembly of sophisticated molecular materials such as synthetic bilayer membranes, host−guest molecules, photoresponsive molecules, and others. Furthermore, the groups are highly recognized in the area of laser spectroscopy, biosensors, and electron microscopy. One of our established activities was the COE project on the “Design and Control of Advanced Molecular Assembly Systems” from 1996 to 2002. On the basis of these foundations, the 21st Century COE program on the research and education of the “Functional Innovation of Molecular Informatics” through the design and synthesis of molecules with highly functional capabilities, the precise control of molecular assemblies and superstructures, and the sensing and characterization of molecular materials and assemblies was organized by the members of the Department of Applied Chemistry and related faculties at Kyushu University.

Fig. 1 shows a summary of the outline of this program. The 21st Century COE Program attempts to create a new science and technology of “Molecular Informatics”, which is a key concept for the generation of artificial molecular intelligence and molecular robotics in the 21st Century. Three divisions, the Advanced Molecules Division, the Advanced Assemblies Division, and the Advanced Sensing Division were organized in order to ensure the effective advancement of the project. The 22 core faculty members from the Departments of Chemistry and Biochemistry, Materials Physics and Chemistry, Materials Process Engineering, and Chemical Systems & Engineering in the Graduate School of Engineering and the Institute for Materials Chemistry and Engineering joined this program. This special issue contains 20 papers and are categorized in five.

1. Design of nano- and supramolecular structures for “Molecular Informatics”
2. Molecular photonics and electronics
3. Design of nanomaterials for “Molecular Informatics”
4. Bioscience and “Molecular Informatics”
5. Sensing and nanostructure analysis for “Molecular Informatics”

The summary of each category are as follows.

1. Design of nano- and supramolecular structures for “molecular informatics”: Suzuki et al. demonstrate the formation of one-dimensional (1D) supramolecular assemblies of small organic compounds aligned by a template polymer. In fact, complexation of linear poly(trimethyleniminium) salts and benzoxazylpyridine (bzpybox) ligands yields the linear supramolecular assemblies on a mica surface by electrostatic interaction. Carbon nanotubes have been at the forefront of nanoscience and nanotechnology; however, because of the insolubility of the nanotubes in solvents, chemical, biochemical and biological applications of these materials have been rather limited. Nakashima reviews his approaches to obtain individually dissolved single-walled carbon nanotubes using synthetic and biological compounds carrying condensed aromatic compounds, and summarizes their fundamental properties. Kobayashi et al. demonstrate the preparation of a polymer brush on a Si-wafer and metal oxide nanoparticles through controlled radical polymerization from an immobilized initiator and suggest that their results will provide useful guidelines for the future design of polymer brushes or polymer/inorganic hybrid materials applicable for molecular informatics. The final paper in this category, presented by Kuroiwa et al. describes supramolecular solvatochromism, the effect of solvents on the self-assembly and charge transfer absorption
characteristics of lipid-packaged, linear mixed-valence platinum complexes.

2. Molecular photonics and electronics: Nagamura et al. describe ultrafast photoresponsive materials and molecular photonics by guided wave mode geometry. Yonemura et al. examine the magnetic field effects on photoelectrochemical reactions of photosensitive electrodes modified with C60-phenothiazine nanoclusters aiming toward the development of nanodevices where photofunctions are controllable using a magnetic field. Horita et al. demonstrate that it is possible to control the morphology and distribution of second-phase particles using severe plastic deformation (SPD) by applying it to Al alloys; in fact, precipitated particles are severely deformed or fragmented by the shear strain introduced by equal-channel angular pressing.

3. Design of nanomaterials for ‘molecular informatics’: Hisaeda et al. report on the preparation of a hybrid nanomaterial using human serum albumin (HSA) and vitamin B12 derivatives, where the incorporation of hydrophobic vitamin B12 derivatives, which have ester groups in place of the peripheral amide moieties of the natural cobalamin, into HSA is primarily controlled by the hydrophobicity of the peripheral ester groups. Enomoto et al. describe the preparation of a series of colloidal crystal (opal) films from variously monodispersed silica spheres on the basis of their recent proposal that the aging of starting solutions for ceramic nanoparticle synthesis can be a factor in controlling the nucleation of the nanoparticles. Ishihara et al. investigate the hydrogen storage property of a Si–carbon nanotube composite that was prepared by the decomposition of tetramethyilsilane using a Ni catalyst. The obtained Si–carbon nanotube composite showed a relatively large hydrogen storage capacity of 2.5 wt%.

4. Bioscience and ‘Molecular Informatics’: Mochizuki et al. report on the preparation of hyaluronan (hyaluronic acid (HA))–ovalbumin (OVA) conjugates by reductive amination between the reducing end of HA and the amino groups of OVA. Their in vivo study using mice suggests that the pretreatment with HA–OVA conjugate considerably reduces the immunogenic activity of native OVA. HA is an attractive biomaterial for modifying not only immunological properties, but also various information of proteins. Nakashima et al. demonstrate the solubilization of an enzyme in a variety of ionic liquids (ILs) by chemical modification of the enzyme using comb-shaped [poly(ethylene glycol)] (PM13). The PM13- modified lipase, PM13-CRL, dissolved in ILs exhibited...
remarkably high activity in all the ILs, whereas unmodified native lipase showed little activity. Comb-shaped PM$_{13}$ was found to be a promising modifier. Shigaki et al. present an approach for the convenient and sensitive evaluation of intracellular protein kinase signals by mass spectroscopy. The method is based on a class of new peptide reagents and MALDI-TOF mass spectrometry. They evaluated activity changes in protein kinase A with dosages of various pharmacological drugs into PC-12 cells and found that the activity changes have a strong correlation with the results of CREB-regulated gene expression. Motoooka et al. carried out molecular-orbital calculations of the four bases of DNA as well as a dimer, dApA, and the calculated results generally reproduced the experimental UPS spectra. They also demonstrated that the alignment of DNA can be controlled by one-dimensional (1D) lattices on Si(100) substrates through capillary action.

5. Sensing and nanostructure analysis for “molecular informatics”: Imasaka’s group report on an autocorrelator for the measurement of a quasi-continuous-wave laser beam sinusoidally modulated at 17 THz and a laser fluorescence spectrometer for the lifetime measurement of dibenzofuran and monochlorodibenzofuran. Then, Nakano et al. report on the application of enzymatically prepared PHQ as a polymer-coated electrode and show that the PHQ electrode is applicable for DNA immobilization by using the Michael reaction on the PHQ-electrode surface. Their system should be important as the basis of a DNA hybridization sensor that enables a totally label-free electrochemical detection of the target DNA. The final paper, presented by Kaneko et al. describes the application of 3D electron tomography using bright-field imaging to clarify the morphologies and the distributions of Si phases precipitated from an Al–Si alloy system.

The Kyushu University COE Program focuses not only on research, but also on educational programs. Two unique programs for establishing a new science of “Molecular Informatics” have been launched for graduate students at the four departments of the graduate school. Fig. 2 shows a summary of the outline of the educational project. The aim of the Core Education Program is to introduce common curricula formed by eliminating barriers among the four different departments of the graduate school involved. The Advanced Education Program consists of three educational groups: (1) The Project Education Cluster; (2) The International Education Cluster; and (3) The Liaison Education Cluster. In the Project Education Cluster, efforts have been made to promote the original research of graduate students through the proposals of research projects by the student themselves. These research projects have been funded by this program. Discussion meetings among students and faculty members of this program have been held. The International Education Cluster has promoted cooperation between researchers of this group and young researchers including graduate students.
students from other Asian countries. An English education program run by a native speaker has been introduced in order to improve researchers’ communication and presentation skills. The Liaison Education Cluster encourages the collaboration between the university and industries. By introducing these systems, we believe that the students in this program can gain a wide perspective not only from the industrial, but also an international point of view. The assessment and planning of this educational program has been carried out by the Assessment and Planning Group.

We hope that the readers of this special issue will recognize the research and educational achievements of our COE program.

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