of compound 2 and metal cations constructed more large channelshaped network. On the other hand, triple helicate 3 was connected by coordination with metal cations to form a 1-D infinite chain. Chirality of each chain was derived from the helicity of the block molecules.



Keywords: helical macromolecules, porous materials, structures of metalloorganic complexes

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Self assembled hierarchical nanostructures: Controlling morphology and molecular arrangement

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An aromatic dipeptide consisting of the two covalently linked phenylalanine units (FF dipeptide), a key structural motif of Alzheimer's beta-amyloid polypeptide, has been reported to form well-defined nanotubes (NTs) and nanowires (NTs). Despite the enormous interest for their properties and applications, however, the link between the nanoscale morphology (NWs or NTs) and the molecular arrangement has been missing. Here, we demonstrate that both NT and NW morphologies of self-assembled dipeptides interconverted by adjusting the preparing conditions. In addition, we also provide the link between the nanoscale morphology (NWs or NTs) and the molecular arrangement of FF diepeptides. Structural analysis via Rietveld refinement of powder x-ray diffraction patterns show that the molecular arrangements of two different morphology, NWs and NTs, display considerable differences in terms of intermolecular hydrogen bond.

Keywords: peptides, nanotubes, powder X-ray diffraction

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X-ray diffraction and small angle X-ray scattering study under high voltage in EHD

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Electro hydrodynamics(EHD) phenomenon is well known to be convections of dielectric liquids under the applied voltage. For instance, EHD actuators are designed for cooling system[1]. Nevertheless, few studies associating with molecular aggregations are reported.Here, it is considered that microscopic clusters under high voltage have a relation with macroscopic mechanism of EHD fluids.Dielectric liquids were C₃F₇OCH₃, C₄F₉OCH₃, C₄F₉OC₂H₅, and C₆F₁₃OCH₃ In-situ observations under high voltage were performed by X-ray diffraction(XRD) and small angle X-ray scattering(SAXS).Data were collected using 18 kW X-ray generator. The wavelength was 0.1542nm. transmission geometry was selected for the measurements.In general, pumping mechanism is divided into ion drag(high current region) and polarization(low current region) pumping. By Fourier transform of XRD, radial distribution function(RDF) is calculated. At 0kV, RDF decreases with increasing molecular weight, M.Also, the intermolecular distance becomes longer at larger M.By *in-situ* observations, the significant point is found. RDF decreased below 5kV(polarization region), though RDF increased above 5kV(ion drag region). Certainly, current density showed the non-linearity at 5kV.In SAXS experiments, scattered intensities were constant below 5kV. In contract, time dependence of the intensities was observed above 5kV. There is a tendency that the size of density fluctuations is inverse proportional to M.It is found that molecular aggregation is caused in ion drag region, While each molecule flows independently in polarization pumping. [1] J.Darbi and K.Ekula, Microelectro. J. 34 (2003) 1067-1074

Keywords: SAXS, pair distribution function, molecules

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Control of stoichiometry and structure: Mechanism of cocrystal formation in mechanochemical synthesis

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Recent years have seen a rapid progress in the synthesis of supramolecular materials by cocrystallisation. The ability to construct cocrystals following a design based on supramolecular synthons allows controlled and predictable synthesis of new forms of materials with improved physicochemical properties. Several methods of cocrystal synthesis and screening are available including solution crystallisation and solid-state grinding. Our group has been investigating solid-state grinding as an advanced method to control polymorphism and stoichiometric diversity in cocrystals. In this contribution, we will delineate our recent conclusions on the supramolecular mechanism of cocrystal formation by grinding. This will focus on the effects of the competition and hierarchy of supramolecular synthons in the course of mechanochemical synthesis. As model compounds, we have explored cocrystals of nicotinamide with dicarboxylic acids that can exhibit the competition between acid-pyridine, acid-acid, acid-amide and amide-pyridine supramolecular synthons. In addition, we also present a qualitative comparison of liquid-assisted grinding to other mechanochemical and non-mechanochemical synthetic approaches, such as neat grinding, thermal methods and solution growth in terms of screening efficiency and stoichiometric diversity.

Keywords: cocrystals, mechanochemical synthesis, stiochiometric diversity