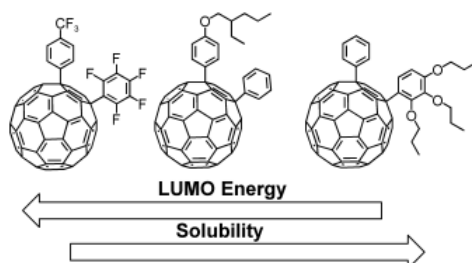


- 1,4-Fullerene Derivatives: Tuning the Properties of the Electron Transporting Layer in Bulk-Heterojunction Solar Cells

Varotto, A.; Treat, N. D.; Jo, J.; Shuttle, C. G.; Batara, N. A.; Brunetti, F. G.; Seo, J. H.; Chabinyk, M. L.; Hawker, C. J.; Heeger, A. J.; Wudl, F. *Angew. Chem. Int. Ed.* **2011**, *50*, 5166–5169.

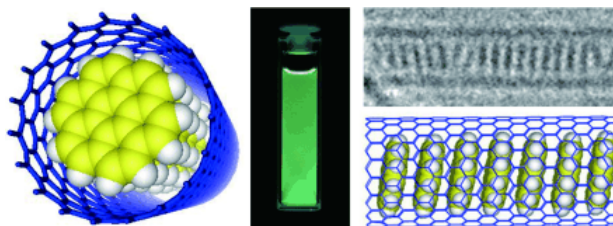
Abstract:



**Tune me up:** The increasing number of new donor materials for organic solar cells requires compatible electron acceptors. A series of 1,4-fullerene adducts with tunable chemical, electronic, and material properties is introduced to effectively influence the photovoltaic characteristics of solar cells.

- Coaxially Stacked Coronene Columns inside Single-Walled Carbon Nanotubes
- Okazaki, T.; Iizumi, Y.; Okubo, S.; Kataura, H.; Liu, Z.; Suenaga, K.; Tahara, Y.; Yudasaka, M.; Okada, S.; Iijima, S. *Angew. Chem. Int. Ed.* **2011**, *50*, 4853–4857.

Abstract:

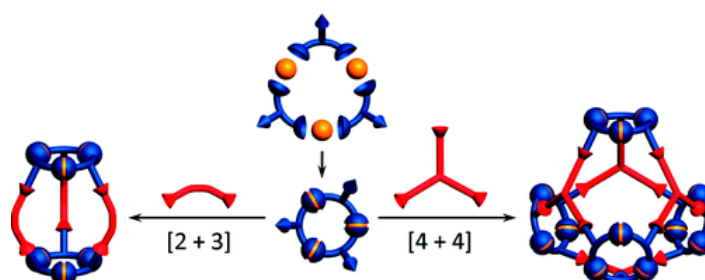


**Pancakes in tubes:** Coronenes, a class of planar  $\pi$ -conjugated molecules, organize in 1D structures when using single-walled carbon nanotubes (SWCNTs) as templates (see picture). Coronene columns with coaxial stacking in SWCNTs exhibit characteristic fluorescence spectra that significantly differ from those of isolated coronene molecules and three-dimensional crystals and that are related to their well-ordered 1D structure.

- Connection of Metallamacrocycles via Dynamic Covalent Chemistry: A Versatile Method for the Synthesis of Molecular Cages

Granzhan, A.; Schouwey, C.; Riis-Johannessen, T.; Scopelliti, R.; Severin, K. *J. Am. Chem. Soc.* **2011**, *133*, 7106-7115.

Abstract:

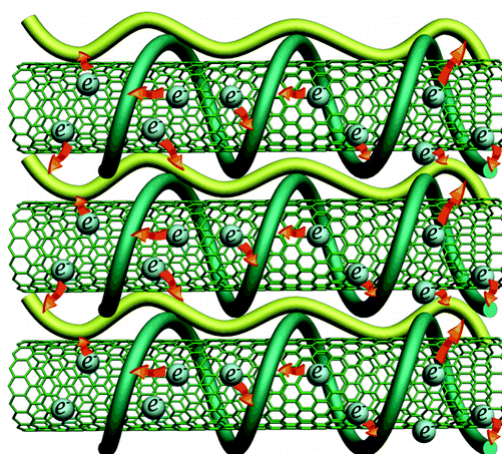


A modular approach for the synthesis of cage structures is described. Reactions of  $[(\text{arene})\text{RuCl}_2]_2$  [arene = p-cymene, 1,3,5-C<sub>6</sub>H<sub>3</sub>Me<sub>3</sub>, 1,3,5-C<sub>6</sub>H<sub>3</sub>(i-Pr)<sub>3</sub>] with formyl-substituted 3-hydroxy-2-pyridone ligands provide trinuclear metallamacrocycles with pendant aldehyde groups. Subsequent condensation reactions with di- and triamines give molecular cages with 3, 6, or 12 Ru centers in a diastereoselective and chemoselective (self-sorting) fashion. Some of the cages can also be prepared in one-pot reactions by mixing  $[(\text{arene})\text{RuCl}_2]_2$  with the pyridone ligand and the amine in the presence of base. The cages were comprehensively analyzed by X-ray crystallography. The diameter of the largest dodecanuclear complex is 3 nm; the cavity sizes range from 290 to 740 Å<sup>3</sup>. An amine exchange process with ethylenediamine allows the clean conversion of a dodecanuclear cage into a hexanuclear cage without disruption of the metallamacrocyclic structures.

- Transparent Conductors from Carbon Nanotubes LBL-Assembled with Polymer Dopant with  $\pi$ - $\pi$  Electron Transfer

Zhu, J.; Shim, B. S.; Di Prima, M.; Kotov, N. A. *J. Am. Chem. Soc.* **2011**, *133*, 7450-7460.

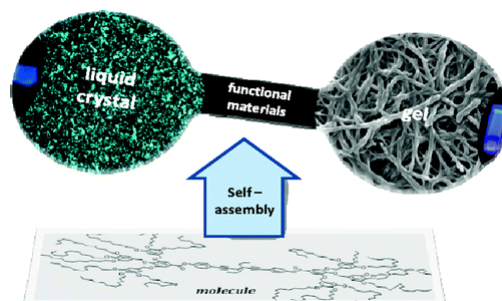
Abstract:



Single-walled carbon nanotube (SWNT) and other carbon-based coatings are being considered as replacements for indium tin oxide (ITO). The problems of transparent conductors (TCs) coatings from SWNT and similar materials include poor mechanical properties, high roughness, low temperature resilience, and fast loss of conductivity. The simultaneous realization of these desirable characteristics can be achieved using high structural control of layer-by-layer (LBL) deposition, which is demonstrated by the assembly of hydroethyl cellulose (HOCS) and sulfonated polyetheretherketone (SPEEK)-SWNTs. A new type of SWNT doping based on electron transfer from valence bands of nanotubes to unoccupied levels of SPEEK through  $\pi$ - $\pi$  interactions was identified for this system. It leads to a conductivity of  $1.1 \times 10^5$  S/m at 66 wt % loadings of SWNT. This is better than other polymer/SWNT composites and translates into surface conductivity of 920  $\Omega$ / and transmittance of 86.7% at 550 nm. The prepared LBL films also revealed unusually high temperature resilience up to 500 °C, and low roughness of 3.5 nm (ITO glass -2.4 nm). Tensile modulus, ultimate strength, and toughness of such coatings are  $13 \pm 2$  GPa,  $366 \pm 35$  MPa, and  $8 \pm 3$  kJ/m<sup>3</sup>, respectively, and exceed corresponding parameters of all similar TCs. The cumulative figure of merit,  $\Pi$ TTC, which included the critical failure strain relevant for flexible electronics, was  $\Pi$ TTC = 0.022 and should be compared to  $\Pi$ TTC = 0.006 for commercial ITO. Further optimization is possible using stratified nanoscale coatings and improved doping from the macromolecular LBL components.

- Control of Self-Assembly of a 3-Hexen-1,5-diyne Derivative: Toward Soft Materials with an Aggregation-Induced Enhancement in Emission  
Pérez, A.; Serrano, J. L.; Sierra, T.; Ballesteros, A.; de Saà, D.; Barluenga, J. *J. Am. Chem. Soc.* **2011**, *133*, 8110–8113.

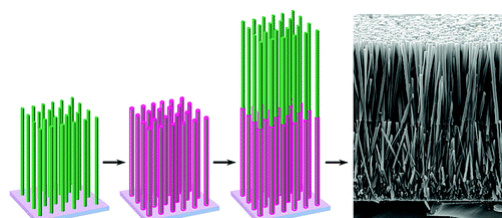
Abstract:



The supramolecular architectures of a fluorophore are controlled through the design of a conjugated polycatenar molecule, the self-assembly of which can be addressed toward a columnar liquid-crystalline phase and organogels. Thus, depending on the environmental conditions for self-assembly, compound **CA9** organizes into an unprecedented hexagonal columnar mesophase in the condensed state, in which half a molecule constitutes the slice of the column, or into a rectangular mesomorphic-like organization in the presence of apolar solvents such as cyclohexane and dodecane, at a concentration in which fibers form and gelling conditions are fulfilled. In this Col<sub>h</sub>-type arrangement, the organization within the columns depends on the solvent. All of the materials prepared show luminescence, and moreover, a remarkable 3-fold increase in fluorescence intensity was observed in going from the solution to the gel state.

- Multilayer Assembly of Nanowire Arrays for Dye-Sensitized Solar Cells  
Xu, C.; Wu, J.; Desai, U. V.; Gao, D. *J. Am. Chem. Soc.* **2011**, *133*, 8122–8125.

Abstract:

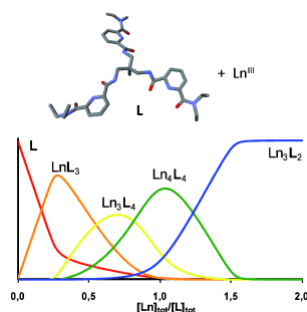


Vertically ordered nanostructures synthesized directly on transparent conducting oxide have shown great promise for overcoming the limitations of current dye-sensitized solar cells (DSCs) based on random networks of nanoparticles. However, the synthesis of such structures with a high internal surface area has been challenging. Here we demonstrate a convenient approach that involves alternate cycles of nanowire growth and self-assembled monolayer coating processes for synthesizing multilayer assemblies of ZnO nanowire arrays and using the assemblies for fabrication of DSCs. The assembled multilayer ZnO nanowire arrays possess an internal surface area that is more than 5 times larger than what one can possibly obtain with single-layer nanowire arrays. DSCs fabricated using such multilayer arrays yield a power conversion efficiency of 7%, which is comparable to that of TiO<sub>2</sub> nanoparticle-based DSCs. The ordered structure with a high internal surface area opens up opportunities for further improvement of DSCs.

- Thermodynamics, Structure and Properties of Polynuclear Lanthanide Complexes with a Tripodal Ligand: Insight into their Self-Assembly

Hamacek, J.; Besnard, C.; Penhouet, T.; Morgantini, P. Y. *Chem. Eur. J.* **2011**, *17*, 6753-6764.

Abstract:

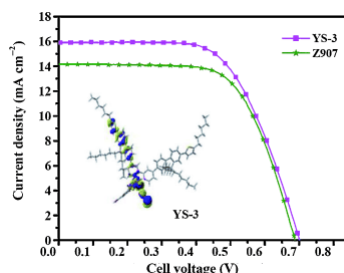


Self-assembly processes between a tripodal ligand and LnIII cations have been investigated by means of supramolecular analytical methods. At an equimolar ratio of components, tetranuclear tetrahedral complexes are readily formed in acetonitrile. The structural analysis of the crystallographic data shows a helical wrapping of binding strands around metallic cations. The properties of this series of highly charged 3D compounds were examined by using NMR spectroscopy and optical methods in solution and in the solid state. In the presence of excess metal, a new trinuclear complex was identified. The X-ray crystal structure elucidated the coordination of metallic cations with two ligands of different conformations. By varying the metal/ligand ratio, a global speciation of this supramolecular system has been evidenced with different spectroscopic methods. In addition, these rather complicated equilibria were successfully characterised with the thermodynamic stability constants. A rational analysis of the self-assembly processes was attempted by using the thermodynamic free energy model and the impact of the ligand structure on the effective concentration is discussed.

- Heteroleptic Ruthenium Sensitizers That Contain an Ancillary Bipyridine Ligand Tethered with Hydrocarbon Chains for Efficient Dye-Sensitized Solar Cells

Yen, Y. S.; Chen, Y. C.; Hsu, Y. C.; Chou, H. H.; Lin, J. T.; Yin, D. J. *Chem. Eur. J.* **2011**, *17*, 6781-6788.

Abstract:

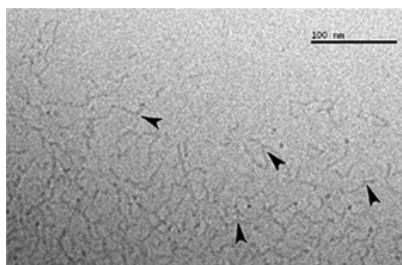


New heteroleptic ruthenium complexes have been synthesized and used as the sensitizers for dye-sensitized solar cells (DSSCs). The ancillary bipyridine ligand contains rigid aromatic segments (fluorene-, carbazole-, or dithieno[3,2-*b*:2',3'-*d*]pyrrole-substituted bipyridine) tethered with a hydrophobic hexyl substituent. The conjugated aromatic segment results in significant bathochromic shift and hyperchromic effects in these complexes compared with Z907 (*cis*-[RuLL'(NCS)<sub>2</sub>]; L=4,4'-dicarboxylic acid-2,2'-bipyridine, L'=4,4'-dinonyl-2,2'-bipyridine). The long hydrocarbon chains help to suppress the dark current if appropriately disposed. DSSCs that use these complexes exhibit very impressive conversion efficiencies (5.94 to 6.91%) that surpass that of Z907-based (6.36%) DSSCs

and are comparable with that of N719-based standard cells (7.13%; N719=*cis*-di(thiocyanato)bis(2,2'-bipyridyl-4,4'-dicarboxylato)ruthenium(II) bis(tetrabutylammonium)) fabricated and measured under similar conditions (active area: 0.5×0.5 cm<sup>2</sup>; AM 1.5 sunlight).

- Self-assembling drugs: A new therapeutic strategy  
Hassan, N.; Ruso, J.; González-Pérez, A. *Soft Matter* **2011**, 7, 5194-5199.

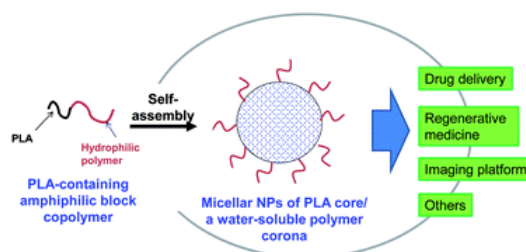
Abstract:



In the current work we proposed the new idea of “self-assembled drug” based on the combination of two or more drugs. As model system we used hexadecyldimethylammonium bromide: dicloxacilin at room temperature. The two drugs are well known for their therapeutic effect and together form worm-like micelles with the combined therapeutic effect of both individual compounds. The system was investigated using, density and sound velocity, dynamic light scattering and cryo- electron microscopy (cryo-TEM) and UV for a complete physicochemical and stability characterization.

- Polylactide (PLA)-based amphiphilic block copolymers: synthesis, self-assembly, and biomedical applications  
Oh, J. *Soft Matter* **2011**, 7, 5096-5108.

Abstract:

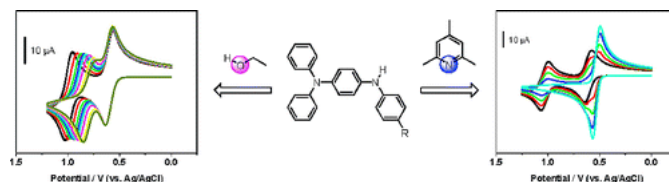


Polylactide (PLA) and its copolymers are one type of hydrophobic aliphatic polyester based on hydroxyalkanoic acids. They possess exceptional qualities: biocompatibility; FDA approval for clinical use; biodegradability by enzyme and hydrolysis under physiological conditions; low immunogenicity; and good mechanical properties. These critical properties have facilitated their value as sutures, implants for bone fixation, drug delivery vehicles, and tissue engineering scaffolds in pharmaceutical and biomedical applications. However, the hydrophobicity of PLA and its copolymers remains concerns for further biological and biomedical applications. One promising approach is to design and synthesize well-controlled PLA-based amphiphilic block copolymers (ABPs); typical hydrophilic copolymers include poly(meth)acrylates, poly(ethylene glycol), polypeptides, polysaccharides, and polyurethanes. This review summarizes recent advances in the synthesis and self-assembly of PLA-containing ABPs and their bio-related applications including drug delivery and imaging platforms of self-assembled nanoparticles, and tissue engineering of crosslinked hydrogels.

- Redox Potential Inversion by Ionic Hydrogen Bonding between Phenylenediamines and Pyridines

Chung, Y. C.; Tu, Y.-J.; Lu, S.-H.; Hsu, W.C.; Chiu, K. Y.; Su, Y. O. *Org. Lett.* **2011**, *13*, 2826–2829.

Abstract:

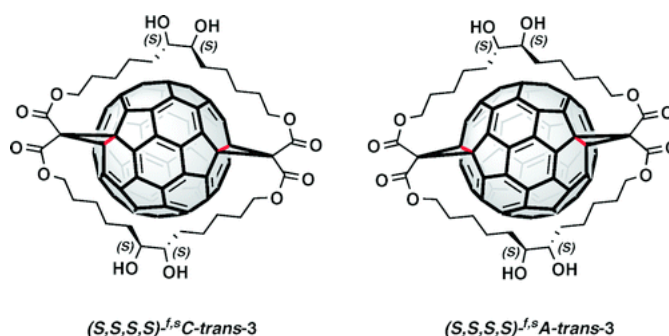


In electrochemical oxidations, the second oxidation potential of phenylenediamines (PD) varies because of hydrogen-bonding formation for PD<sup>•+</sup> with pyridines. A linear relationship was obtained for the potential shift as a function of pK<sub>a</sub> of the protonated pyridines and potential inversion could be observed. The oxidized PD<sup>•+</sup> could also form hydrogen bonding with alcohols and the shift of potential exhibits a different pattern.

- A Facile Access to Enantiomerically Pure [60]Fullerene Bisadducts with the Inherently Chiral *Trans*-3 Addition Pattern

Riala, M.; Chronakis, N. *Org. Lett.* **2011**, *13*, 2844–2847.

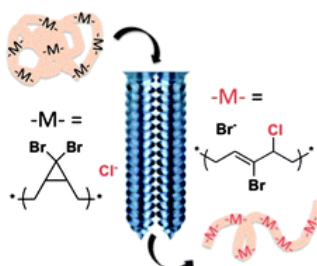
Abstract:



The Bingel reaction between C<sub>60</sub> and an enantiopure bismalonate tether equipped with two acetonide moieties led to the synthesis and successful column chromatographic isolation of the enantiomerically pure *f,sC* and *f,sA* bisadducts with the inherently chiral *trans*-3 addition pattern. Acidic deprotection of the acetonide groups gave access to novel chiral fullerene compounds which combine the inherent chirality of the fullerene core with the functional glycol groups located on the tether.

- Mechanochemically triggered bond formation in solid-state polymers

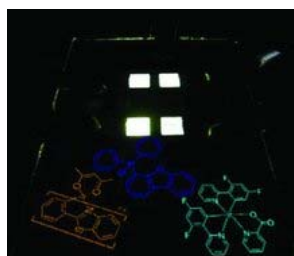
Abstract:



Polybutadiene was functionalized with dibromo-, dichloro-, and bromochloro-carbene to give *gem*-dihalocyclopropanated (*g*DHC) polymers, in which the *g*DHCs act as mechanically activated functional groups or mechanophores. The polymers were extruded to determine the mechanophore activity in the solid state. The extent of *g*DHC ring opening depends on both the polymer composition and the macroscopic shear stress, ranging from 6.0% to over 30% after an hour of extrusion. In addition, the 2,3-dibromoalkene formed from mechanical activation of the *gem*-dibromocyclopropane was found to undergo subsequent nucleophilic substitution by chloride in the solid state. The number of solid-state substitution reactions far exceeds the number of main-chain bonds broken, a finding with implications for the future use of mechanophores in self-strengthening or self-healing polymers.

- A Single Phosphine Oxide Host for High-Efficiency White Organic Light-Emitting Diodes with Extremely Low Operating Voltages and Reduced Efficiency Roll-Off  
Han, C.; Xie, G.; Xui, H. ; Zhang, Z. ; Xie, L. ; Zhao, Y.; Liu, S.; Huang, W. *Adv. Mater.* **2011**, *23*, 2491-2496.

Abstract:



**Highly efficient white organic light-emitting diodes (WOLEDs) with a simple, single-host-based structure** are fabricated to realize the state-of-the-art performance of extremely low driving voltages, high efficiencies, and low efficiency roll-offs. This is the first single-host-based WOLED with both high efficiency and extremely low operating voltage at practical luminescence, demonstrating the great potential of these WOLEDs for portable display and lighting applications.