

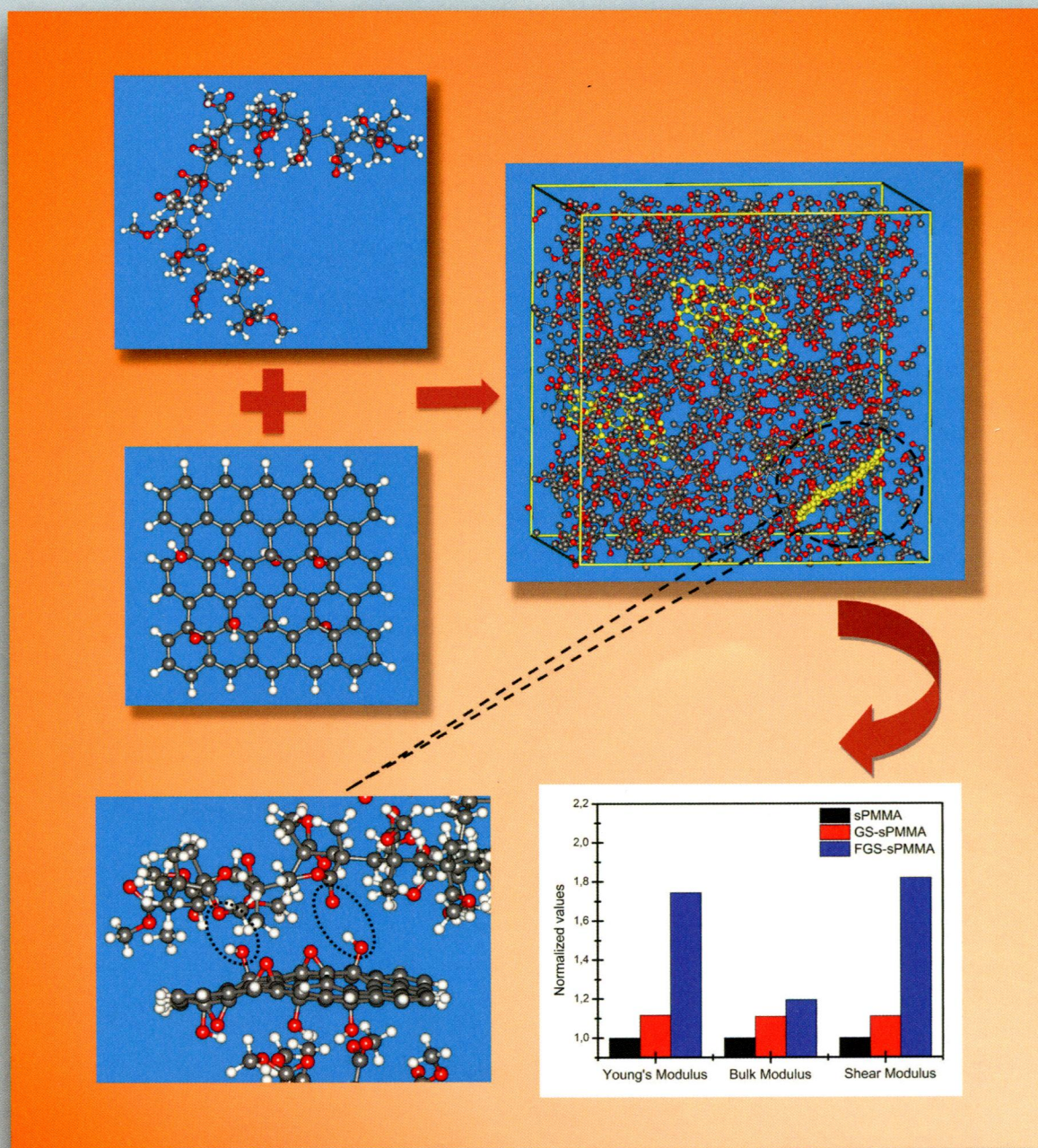
Macromolecules

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ON THE COVER: According to recent experimental studies, introducing oxygen-containing functional groups in graphene sheets can greatly enhance the mechanical properties of their nanocomposites with polar polymers even at extremely low loadings. The graphic shows a schematic of such a functionalized graphene sheet (FGS) with 5 hydroxyl groups and 3 oxygen atoms on its surface, a typical configuration of a 15-monomer-long syndiotactic poly(methyl methacrylate) (sPMMA) chain, and an atomistic snapshot of a FGS-sPMMA model nanocomposite system containing 27 sPMMA chains and 3 FGS (6.54 wt % loading) in a cell with dimensions $(40 \times 40 \times 40) \text{ \AA}^3$ subject to periodic boundary conditions. With this model system and the help of statistical mechanics and statistical thermodynamics, one can simulate the mechanical properties of the nanocomposite in full atomistic detail and carry out a comparative study of the effect of graphene functionalization on the degree of mechanical reinforcement. The simulations demonstrate that adding just 6.54 wt % FGs in the host matrix results in an improvement of the Young's modulus E by $\sim 74\%$, of the bulk modulus B by $\sim 19\%$, and of the shear modulus G by 83% . An important contributor to this large property enhancement is the hydrogen bonds formed between FGS and surrounding sPMMA chains. In the image, we can observe the formation of two hydrogen bonds with the same sPMMA chain on the one side of the FGS (there is a third hydrogen bond with a different chain on the other side of the sheet). See *Macromolecules* **2014**, *47* (22), 8072–8088.

Articles

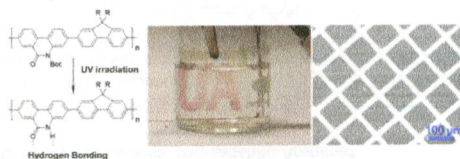
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Patternable Conjugated Polymers with Latent Hydrogen-Bonding on the Main Chain

Kun Yang, Tianda He, Xiaoyi Chen, Stephen Z. D. Cheng, and Yu Zhu*



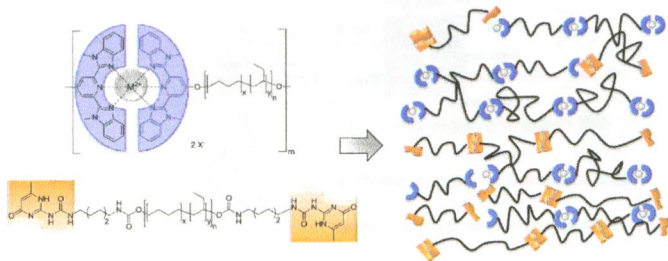
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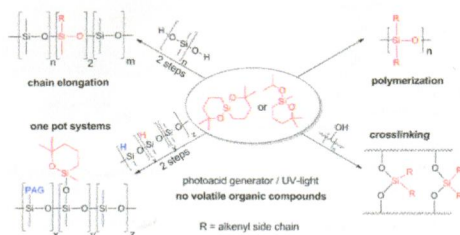
Supramolecular Polymers with Orthogonal Functionality

Souleymane Coulibaly, Christian Heinzmann, Frederick L. Beyer, Sandor Balog, Christoph Weder,* and Gina L. Fiore*



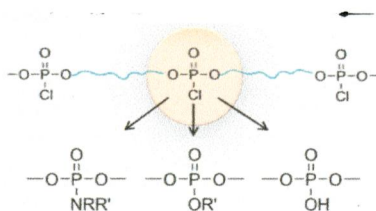
Oxasilacycles Leading to UV-Curable Polymers: Synthesis and Application

Christian A. Anger, Julian Kehrle, Konrad Hindelang, Jonathan G. C. Veinot, Jürgen Stohrer, and Bernhard Rieger*



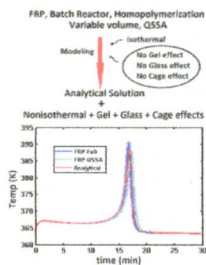
Poly(alkylidene chlorophosphate)s via Acyclic Diene Metathesis Polymerization: A General Platform for the Postpolymerization Modification of Poly(phosphoester)s

Mark Steinmann, Jens Markwart, and Frederik R. Wurm*



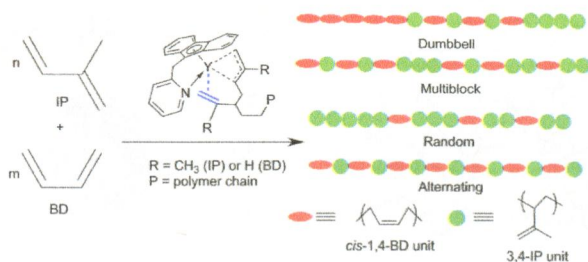
Analytical Solution of Free Radical Polymerization: Applications-Implementing Nonisothermal Effect

Dhiraj K. Garg, Christophe A. Serra,* Yannick Hoarau, Dambarudhar Parida, M. Bouquey, and R. Muller



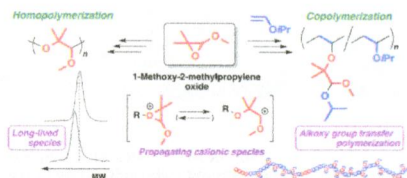
Unprecedented 3,4-Isoprene and *cis*-1,4-Butadiene Copolymers with Controlled Sequence Distribution by Single Yttrium Cationic Species

Bo Liu, Xingbao Wang, Yupeng Pan, Fei Lin, Chunji Wu, Jingping Qu, Yi Luo, and Dongmei Cui*



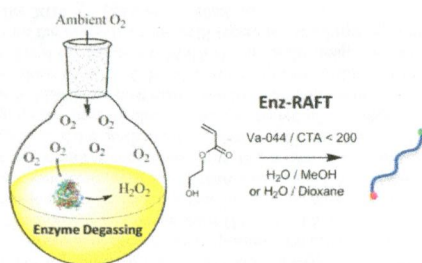
Alkoxyoxirane, a Unique Cyclic Monomer: Controlled Cationic Homopolymerization Mediated by Long-Lived Species and Copolymerization with Vinyl Ether via Alkoxy Group Transfer

Arihiro Kanazawa, Shungo Kanda, Shokyoku Kanaoka, and Sadahito Aoshima*



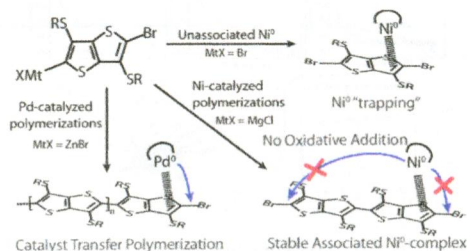
Highly Controlled Open Vessel RAFT Polymerizations by Enzyme Degassing

Robert Chapman, Adam J. Gormley, Karla-Luise Herpoldt, and Molly M. Stevens*

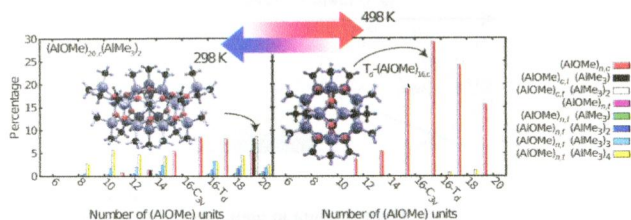


Evidence for Catalyst Association in the Catalyst Transfer Polymerization of Thieno[3,2-*b*]thiophene

Pieter Willot and Guy Koeckelberghs*

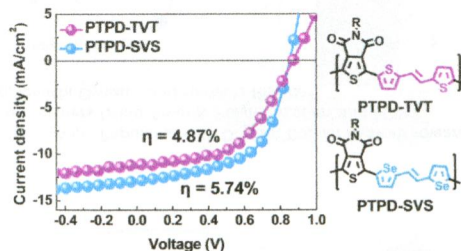
The Dynamic Equilibrium Between $(\text{AlOMe})_n$ Cages and $(\text{AlOMe})_n(\text{AlMe}_3)_m$ Nanotubes in Methylaluminoxane (MAO): A First-Principles Investigation

Zackary Falls, Nina Tymińska, and Eva Zurek*



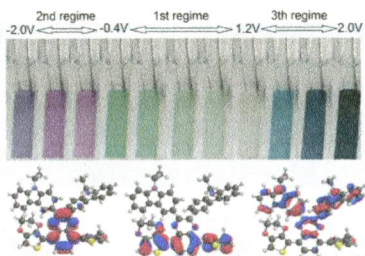
TPD-Based Copolymers with Strong Interchain Aggregation and High Hole Mobility for Efficient Bulk Heterojunction Solar Cells

Ye Rim Cheon, Yu Jin Kim, Jong-jin Ha, Myeong-Jong Kim, Chan Eon Park,* and Yun-Hi Kim*



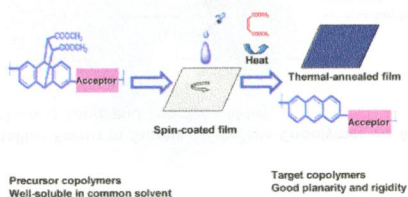
Toward Purple-to-Green-to-Transmissive-to-Black Color Switching in Polymeric Electrochrome

Elif Karabiyik, Emre Sefer, Fatma Baycan Koyuncu, Murat Tonga, Eyüp Özdemir, and Sermet Koyuncu*



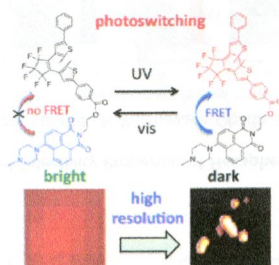
Synthesis of Anthracene-Based Donor–Acceptor Copolymers with a Thermally Removable Group for Polymer Solar Cells

Chunchen Liu, Wenzhan Xu, Xing Guan, Hin-Lap Yip,* Xiong Gong,* Fei Huang,* and Yong Cao



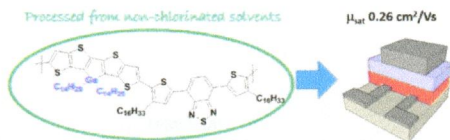
Water-Soluble Polymeric Photoswitching Dyads Impart Super-Resolution Lysosome Highlighters

Chong Li, Zhe Hu, Matthew P. Aldred, Ling-Xi Zhao, Hui Yan, Guo-Feng Zhang, Zhen-Li Huang,* Alexander D. Q. Li,* and Ming-Qiang Zhu*



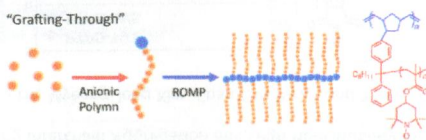
Alternating Copolymers Incorporating Dithienogemolodithiophene for Field-Effect Transistor Applications

Jessica Shaw, Hongliang Zhong, Chin Pang Yau, Abby Casey, Ester Buchaca-Domingo, Natalie Stingelin, David Sparrowe, William Mitchell, and Martin Heeney*



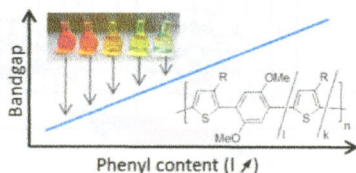
Expanding the Dimensionality of Polymers Populated with Organic Robust Radicals toward Flow Cell Application: Synthesis of TEMPO-Crowded Bottlebrush Polymers Using Anionic Polymerization and ROMP

Takashi Sukegawa, Issei Masuko, Kenichi Oyaizu,* and Hiroyuki Nishide*



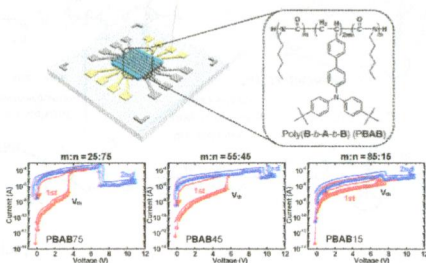
Steering Poly(thiophene) Properties by Incorporation of Phenyl Groups

Tine Hardeman and Guy Koeckelberghs*



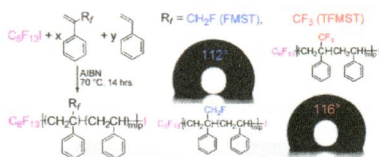
Well-Defined Block Copolymers with Triphenylamine and Isocyanate Moieties Synthesized via Living Anionic Polymerization for Polymer-Based Resistive Memory Applications: Effect of Morphological Structures on Nonvolatile Memory Performances

Beom-Goo Kang, Jingon Jang, Younggul Song, Myung-Jin Kim, Takhee Lee,* and Jae-Suk Lee*



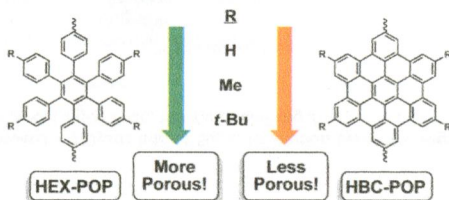
Iodine Transfer Copolymerization of Fluorinated α -Methylstyrenes with Styrene Using 1-Iodoperfluorohexane as the Chain Transfer Agent

Justyna Walkowiak-Kulikowska, Anna Szwajca, Frédéric Boschet, Véronique Gouverneur, and Bruno Ameduri*



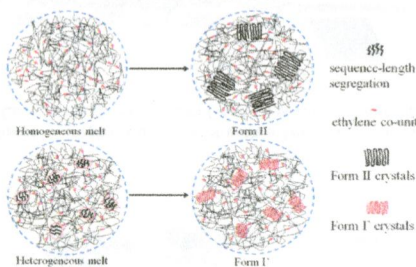
Substituent Effects on the Gas Sorption and Selectivity Properties of Hexaphenylbenzene and Hexabenzocoronene Based Porous Polymers

Christina M. Thompson, Gregory T. McCandless, Sumudu N. Wijenayake, Obada Alfarawati, Mohammad Jahangiri, Atef Kokash, Zachary Tran, and Ronald A. Smaldone*



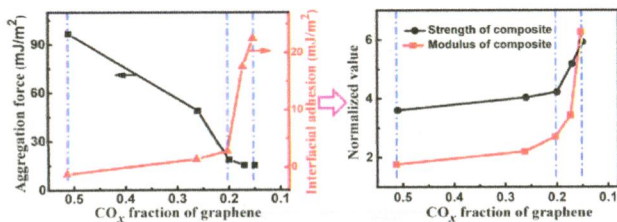
Direct Formation of Different Crystalline Forms in Butene-1/Ethylene Copolymer via Manipulating Melt Temperature

Yao tao Wang, Ying Lu, Jiayi Zhao, Zhiyong Jiang, and Yongfeng Men*



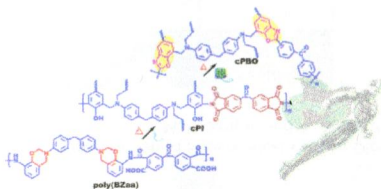
Rational Design of Graphene Surface Chemistry for High-Performance Rubber/Graphene Composites

Zhenghai Tang, Liqun Zhang, Wenjiang Feng, Baochun Guo,* Fang Liu, and Demin Jia



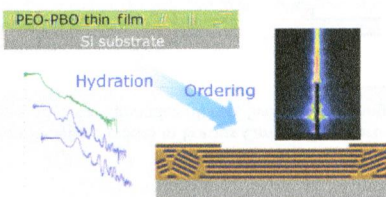
An Ultrahigh Performance Cross-Linked Polybenzoxazole via Thermal Conversion from Poly(benzoxazine amic acid) Based on Smart *o*-Benzoxazine Chemistry

Kan Zhang, Jia Liu, and Hatsuo Ishida*



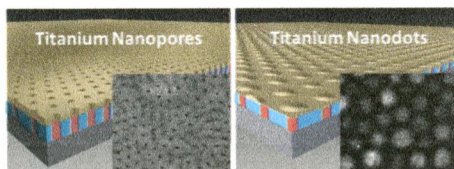
Hydration and Ordering of Lamellar Block Copolymer Films under Controlled Water Vapor

Yohei Kamata,* Andrew J. Parnell, Philipp Gutfreund, Maximilian W. A. Skoda, Andrew J. C. Dennison, Robert Barker, Shaomin Mai, Jonathan R. Howse, Anthony J. Ryan, Naoya Torikai, Masami Kawaguchi, and Richard A. L. Jones



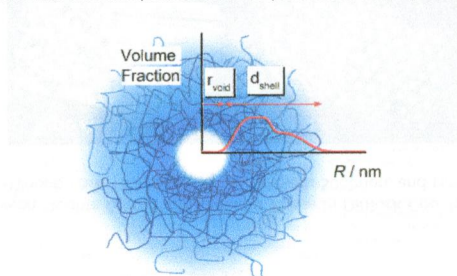
Formation of Titanium Nanostructures on Block Copolymer Templates with Varying Molecular Weights

Martin Kreuzer,* Claudia Simão, Ana Diaz, and Clivia M. Sotomayor Torres



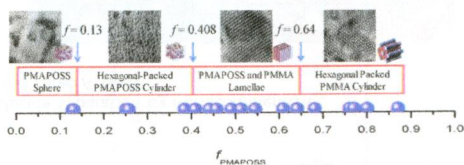
How Hollow Are Thermoresponsive Hollow Nanogels?

Janine Dubbert, Tobias Honold, Jan Skov Pedersen, Aurel Radulescu, Markus Drechsler, Matthias Karg, and Walter Richtering*



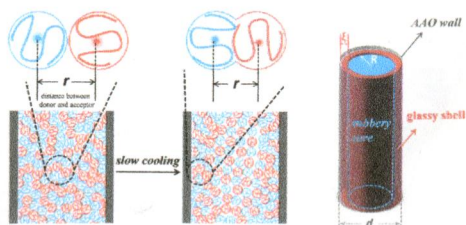
Hydrogen Bond Interactions Mediate Hierarchical Self-Assembly of POSS-Containing Block Copolymers Blended with Phenolic Resin

Chin-Wei Chiou, Yung-Chih Lin, Lei Wang, Rina Maeda, Teruaki Hayakawa, and Shiao-Wei Kuo*



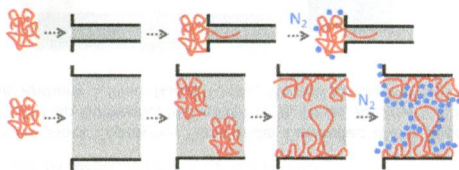
Growth of Polymer Nanorods with Different Core–Shell Dynamics via Capillary Force in Nanopores

Ye Sha, Linling Li, Xiaoliang Wang, Yuanxin Wan, Jie Yu, Gi Xue,* and Dongshan Zhou*



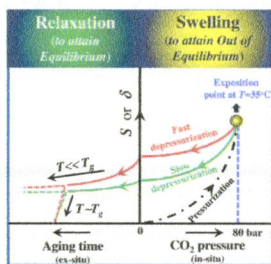
Intercalation and Confinement of Poly(ethylene oxide) in Porous Carbon Nanoparticles with Controlled Morphologies

Fabienne Barroso-Bujans,* Pablo Palomino, Felix Fernandez-Alonso, Svemir Rudić, Angel Alegria, Juan Colmenero, and Eduardo Enciso



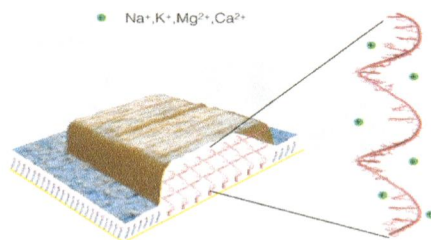
Relaxation of Ultrathin Polystyrene Films Hyperswollen in Supercritical Carbon Dioxide

J. K. Bal, T. Beuvier, M. S. Chebil, G. Vignaud, Y. Grohens, M. K. Sanyal, and A. Gibaud*



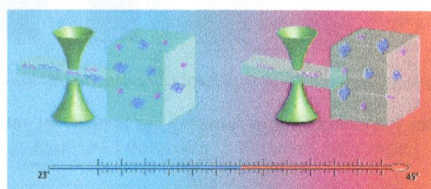
Determination of Average Internucleotide Distance in Variable Density ssDNA Nanobrushes in the Presence of Different Cations Species

Maryse D. Nkoua Ngavouka, Alessandro Bosco, Loredana Casalis,* and Pietro Parisse



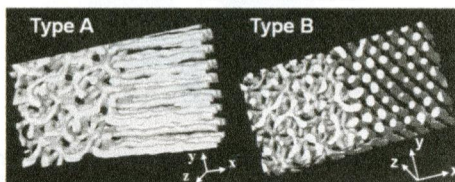
Temperature Driven Macromolecule Separation by Nanoconfinement

Iliaria De Santo, Filippo Causa, and Paolo A. Netti*



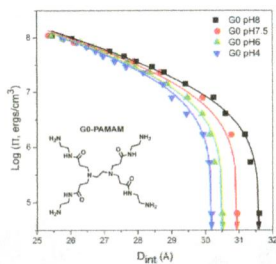
Epitaxial Phase Transition between Double Gyroid and Cylinder Phase in Diblock Copolymer Thin Film

Jueun Jung, Junyoung Lee, Hae-Woong Park, Taihyun Chang,* Hidekazu Sugimori, and Hiroshi Jinnai



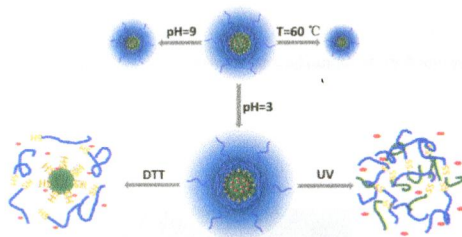
Role of pH on the Compaction Energies and Phase Behavior of Low Generation PAMAM–DNA Complexes

Min An, James M. Hutchison, Sean R. Parkin, and Jason E. DeRouchey*



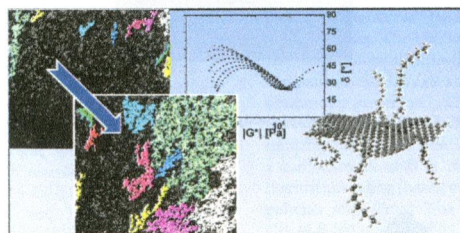
Quadruple-Stimuli-Sensitive Polymeric Nanocarriers for Controlled Release under Combined Stimulation

Ziquan Cao, Hao Wu, Jie Dong, and Guojie Wang*



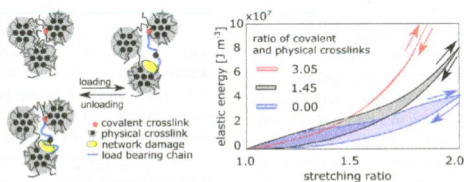
Shear- and Temperature-Induced Graphene Network Evolution in Graphene/Polystyrene Nanocomposites and Its Influence on Rheological, Electrical, and Morphological Properties

F. Beckert, A. Held, J. Meier, R. Mülhaupt, and C. Friedrich*



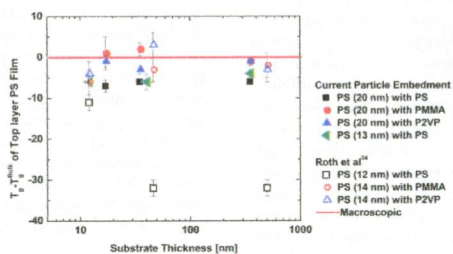
Mechanical Response of Hybrid Cross-Linked Networks to Uniaxial Deformation: A Molecular Dynamics Model

Jan Zidek,* Josef Jancar, Andrey Milchev, and Thomas A. Vilgis



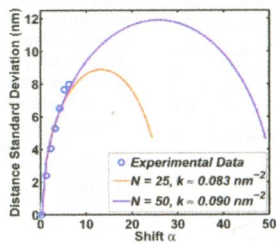
Substrate Effects on Glass Transition and Free Surface Viscoelasticity of Ultrathin Polystyrene Films

Heedong Yoon and Gregory B. McKenna*



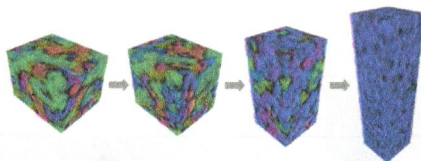
A Landau–Peierls Analysis of Contact Hole Placement in Directed Self-Assembly of Linear Arrays of Block Copolymer Cylinders

Nabil Laachi, David Shykind, and Glenn H. Fredrickson*



Molecular Simulations Shed Light on Supersoft Elasticity in Polydomain Liquid Crystal Elastomers

Gregor Skačej* and Claudio Zannoni

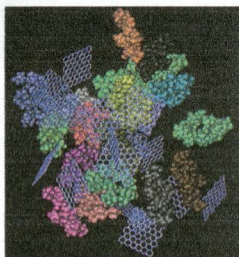


8833

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Graphene/Hyperbranched Polymer Nanocomposites: Insight from Molecular Dynamics Simulations

Kostas Karatasos*



Notes

8846

DOI: 10.1021/ma501921z

Unprecedented Lower Critical Solution Temperature Behavior of Polyimides in Organic Media

Sun Dal Kim, Sang Youl Kim,* and Im Sik Chung*

