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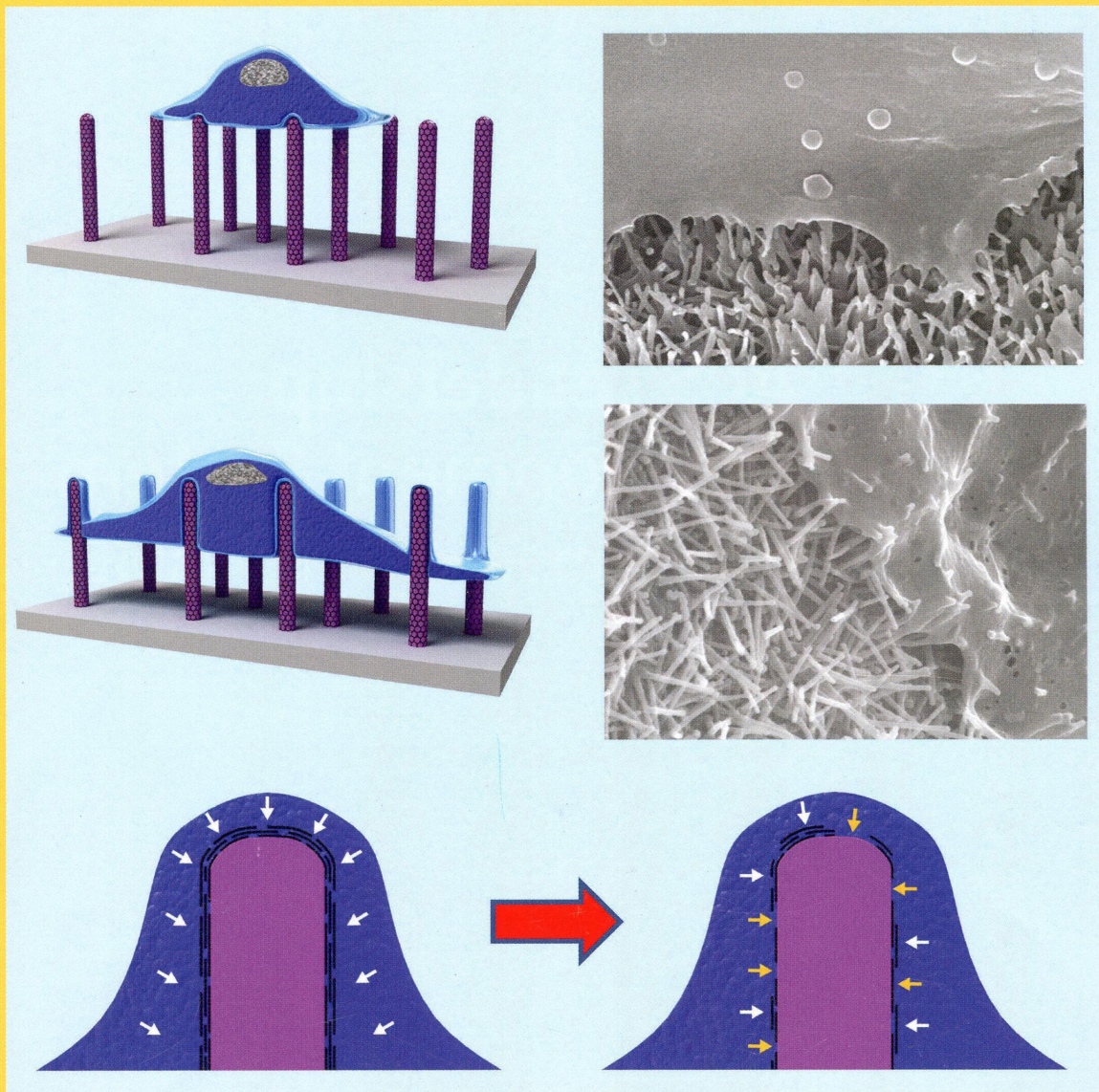
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Programmed Smart
Behavior of SANGs
with a Unique
Core-Shell
Nanostructure for
Osteogenesis
(see page 13849)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: The promotion of osteogenesis by single-crystal apatite nanowires sheathed in graphitic layers (SANGs) is specific to their unique nanotopographic surface chemistry. SANG scaffolds with graphitic layers provided a significantly better supportive structure for the differentiation of human mesenchymal stem cells (hMSCs) into osteoblasts than did single-crystal apatite nanowire (SAN) scaffolds with an apatite surface. The nanotopographic surface structure of SANGs reproduces the conditions in bone tissue, which presents a more alkaline environment rich in ceramic/mineral components. Therefore, the SANG surface graphitic structure is beneficial for the initial growth and differentiation of hMSCs, which would be followed by degradation of graphitic shells, and the bare apatite core would provide a biologically compatible environment for the later stages of osteogenesis. We believe that our SANGs with a unique core–shell nanostructure provide a useful scaffolding material for hMSC-based tissue engineering strategies because they reflect the dynamic nature of many biological processes.

Articles

Biophysical Chemistry and Biomolecules

13777

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Theoretical Analysis of Microtubule Dynamics at All Times

Xin Li and Anatoly B. Kolomeisky*

13785

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Modulation of Non Steroidal Anti-Inflammatory Drug Induced Membrane Fusion by Copper Coordination of These Drugs: Anchoring Effect

Anupa Majumdar, Sreeja Chakraborty, and Munna Sarkar*

13800

DOI: 10.1021/jp5089965

Multiscale Simulations Give Insight into the Hydrogen In and Out Pathways of [NiFe]-Hydrogenases from *Aquifex aeolicus* and *Desulfovibrio fructosovorans*

Francesco Oteri, Marc Baaden, Elisabeth Lojou, and Sophie Sacquin-Mora*

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DOI: 10.1021/jp509398e

Distance Geometry Protocol to Generate Conformations of Natural Products to Structurally Interpret Ion Mobility-Mass Spectrometry Collision Cross Sections

Sarah M. Stow, Cody R. Goodwin, Michal Kliman, Brian O. Bachmann, John A. McLean,* and Terry P. Lybrand*

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DOI: 10.1021/jp510245n

Self-Association of Amphotericin B: Spontaneous Formation of Molecular Structures Responsible for the Toxic Side Effects of the Antibiotic

Joanna Starzyk, Marcin Gruszecki, Krzysztof Tutaj, Rafal Luchowski, Radoslaw Szlajak, Piotr Wasiko, Wojciech Grudzinski, Jacek Czub, and Wieslaw I. Gruszecki*

13833

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DNA Lesion Can Facilitate Base Ionization: Vertical Ionization Energies of Aqueous 8-Oxoguanine and its Nucleoside and Nucleotide

Vladimir Palivec, Eva Pluhařová, Isaak Unger, Bernd Winter, and Pavel Jungwirth*

Biomaterials, Surfactants, and Membranes

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DOI: 10.1021/jp503910r

Effect of Methyl-Branched Fatty Acids on the Structure of Lipid Bilayers

David Poger,* Bertrand Caron, and Alan E. Mark

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DOI: 10.1021/jp5075576

Effect of Graphitic Layers Encapsulating Single-Crystal Apatite Nanowire on the Osteogenesis of Human Mesenchymal Stem Cells

Namjo Jeong, Yun Chang Park, Kyung Mee Lee, Jae Hyup Lee,* and Misun Cha*

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Excited-State Proton Transfer of Photoacids Adsorbed on Biomaterials

Nadav Amdursky, Ron Simkovitch, and Dan Huppert*

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DOI: 10.1021/jp509282h

Molecular Simulation and Experimental Study of CO₂ Absorption in Ionic Liquid Reverse Micelle

Wei Shi,* Lei Hong, Krishnan Damodaran, Hunaid B. Nulwala, and David R. Luebke

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DOI: 10.1021/jp510825b

Irreversible Catalyst Activation Enables Hyperpolarization and Water Solubility for NMR Signal Amplification by Reversible Exchange

Milton L. Truong,* Fan Shi, Ping He, Bingxin Yuan, Kyle N. Plunkett, Aaron M. Coffey, Roman V. Shchepin, Danila A. Barskiy, Kirill V. Kovtunov, Igor V. Koptuyug, Kevin W. Waddell, Boyd M. Goodson, and Eduard Y. Chekmenev*

Liquids; Chemical and Dynamical Processes in Solution

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DOI: 10.1021/jp5060099

Theoretical Insight into the Coordination of Cyclic β -D-Glucose to [Al(OH)(aq)]²⁺ and [Al(OH)₂(aq)]¹⁺ Ions

Meng-Fu He, Hong-Quan Fu, Ben-Fang Su, Hua-Qing Yang,* Jin-Qiang Tang, and Chang-Wei Hu*

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Ab Initio Molecular Dynamics Study of the Mechanism of Proton Recombination with a Weak Base

Jérôme Cuny* and Ali A. Hassanali*

13913  DOI: 10.1021/jp508379w

Ammonium Recognition by 18-Crown-6 in Different Solutions and at an Aqueous Interface: A Simulation Study

G. Benay and G. Wipff*

13930  DOI: 10.1021/jp508950k

Ionic Liquids at Nonane–Water Interfaces: Molecular Dynamics Studies

Sourav Palchowdhury and B. L. Bhargava*

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Polarization versus Temperature in Pyridinium Ionic Liquids

Vitaly V. Chaban* and Oleg V. Prezhdo

13946  DOI: 10.1021/jp510389d

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Jagannath Kuchlyan, Debasis Banik, Arpita Roy, Niloy Kundu, and Nilmoni Sarkar*

13954  DOI: 10.1021/jp509425p

Theoretical Studies of Structure and Dynamics of Molten Salts: The LiF–ThF₄ System

Jian-Biao Liu, Xin Chen, Yi-Heng Qiu, Chao-Fei Xu, W. H. Eugen Schwarz, and Jun Li*

13963  DOI: 10.1021/jp511207s

Understanding Cage Effects in Imidazolium Ionic Liquids by ¹²⁹Xe NMR: MD Simulations and Relativistic DFT Calculations

Giacomo Saielli,* Alessandro Bagno, Franca Castiglione, Roberto Simonutti, Michele Mauri, and Andrea Mele*

Glasses, Colloids, Polymers, and Soft Matter

13969  DOI: 10.1021/jp5086137

Co-Assembled Conductive Hydrogel of *N*-Fluorenylmethoxycarbonyl Phenylalanine with Polyaniline

Priyadarshi Chakraborty, Partha Bairi, Sanjoy Mondal, and Arun K. Nandi*

13981  DOI: 10.1021/jp509061z

Viscosity of Nafion Oligomers as a Function of Hydration and Counterion Type: A Molecular Dynamics Study

Kevin B. Daly, Athanasios Z. Panagiotopoulos, Pablo G. Debenedetti, and Jay B. Benziger*

13992  DOI: 10.1021/jp509760x

Analysis of Solvation and Gelation Behavior of Methylcellulose Using Atomistic Molecular Dynamics Simulations

Wenjun Huang, Indranil S. Dalal, and Ronald G. Larson*