

Editorial

Topology- and Geometry-Controlled Functionalization of Nanostructured Metamaterials

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The study of topological matter is one of the most fascinating areas of modern physics. The present Special Issue is focused on the topology- and complex geometry-driven effects of advanced micro- and nanoarchitectures fabricated of conventional and topologically non-trivial materials. The design, production, and characterization of future quantum devices for light emission, quantum cryptography, quantum information processing, thermoelectric applications, bolometry, and other nanotechnologies are of paramount importance. Correspondingly, high-quality experimental and theoretical research has been conducted to obtain a systematic understanding of their properties, thereby leading to novel applications. This Special Issue brings together experts in the field of the topology- and geometry-controlled functionalization of nanostructured materials of unique technological potential.

Prof. Victor Yu. Timoshenko and his co-authors present halloysite nanotubes (HNTs) with immobilized plasmonic nanoparticles (NPs) for biophotonic applications [1]. HNTs with immobilized gold and silver NPs belong to a class of nanocomposite materials, whose physical properties and applications depend on the geometry of the arrangements of the plasmonic nanoparticles on the HNT surfaces. They explore HNTs:(Au, Ag) NPs as potential nano-templates for surface-enhanced Raman scattering (SERS). The structure and plasmonic properties of the nanocomposites based on the HNTs and Au- and Ag NPs are studied by transmission electron microscopy and optical spectroscopy. The optical extinction spectra of the aqueous suspensions of the HNTs:(Au, Ag) NPs and the spatial distributions of the electric fields are simulated, and the simulation results demonstrate the corresponding localized plasmonic resonances and “hot spots” of the electric field close to those NPs. In vitro experiments reveal an enhancement of the protein SERS in the fibroblast cells with added HNTs: Ag NPs. The optical properties and SERS activity of the nanocomposites based on HNTs and plasmonic NPs are highly promising for applications in biosensorics and biophotonics.

Prof. Osama Saber and his co-authors analyze the enhancement of the supercapacitive performance of cobalt-tin-cyanate layered structures through their conversion from 2D materials into 1D nanofibers [2]. This research was motivated by the search for metal hydroxides with a rational micro-nanomorphology design to achieve overall high-performance electrodes for supercapacitor and energy storage applications. The authors succeeded in obtaining Sn/Co-nanolayered structures with plate and nanofibrous morphologies. Additionally, the plate nanostructures could be transformed into obtain plate-nanofibrous morphologies. In this trend, dual anions such as cyanate and nitrate are applied to intercalate among the nanolayers of the cobalt-tin and act as building blocks or pillars, producing a series of nanolayered structures. The nanolayers of Sn/Co are curled and converted into nanofibers due to the repulsion forces among the intercalated anions. This conversion is confirmed by scanning electron microscopy. In addition, the intercalation reactions and



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nanolayered structures were indicated by X-ray diffraction, thermal analyses, and Fourier-transform infrared spectroscopy. The electrochemical supercapacitive behaviors of the different nanostructures of the Sn/Co hydroxyl double salts and Sn/Co layered double hydroxide, such as the plate, plate-nanofiber, and nanofibrous morphologies, are investigated in a three-electrode assembly system. The results suggest that the nanofiber morphology of the Sn/Co layered double hydroxide exhibit better specific capacitance performances than the other two morphologies do. The enhanced specific capacitance (658 Fg^{-1}) and excellent cyclic stability (89%) of the nanofibers of the Sn/Co layered double hydroxide are attributed to the synergetic effects between the electric double layer capacitive character of tin and the pseudo-capacitance nature of cobalt.

An atomistic study of phonons and thermal transport in Si/SiO₂ multishell nanotubes is presented by Prof. Vladimir M. Fomin and Prof. Denis Nika and their collaborators [3]. The phonon energy spectra are obtained using the atomistic lattice dynamics approach. Thermal conductivity is calculated using the Boltzmann transport equation within the relaxation-time approximation. The redistribution of the vibrational spectra in the multishell nanotubes leads to larger decreases in the phonon group velocity and the thermal conductivity compared to those for the homogeneous Si nanowires. Phonon scattering on the Si/SiO₂ interfaces is another key factor of a strong reduction of the thermal conductivity in these structures (down to $0.2 \text{ Wm}^{-1}\text{K}^{-1}$ at room temperature). Importantly, the phonon thermal transport in the Si/SiO₂ nanotubes is efficiently suppressed by a proper choice of nanotube geometrical parameters: the lateral cross section, thickness, and number of shells. Such nanotubes are perspective for applications in modern electronics in cases when low heat conduction is required.

Dr. Tomasz Kwapiński and Mr. Marcin Kurzyina report on electron pumping and spectral density dynamics in energy-gapped topological chains [4]. Electron pumping through energy-gapped systems is restricted due to the vanishing local density of states at the Fermi level. The authors propose that a topological Su–Schrieffer–Heeger (SSH) chain between the unbiased leads can be an effective electron pump. The electron transport properties of the topologically trivial and nontrivial systems are analyzed in the presence of external time-dependent forces in the form of one-Gaussian or two-Gaussian perturbations (train impulses). The topologically trivial chain is a much better charge pump than the other normal or nontrivial chains are. It is important that, during perturbation, the electrons are pumped through the mid-gap temporary states or through the induced sidebands states outside of the energy gap. The local density of states dynamics are also analyzed during the quench transition between the different topological phases of the SSH chain. After the quench, the edge topological states migrate through the other sites and temporarily exist in a topologically trivial part of the system. These topological materials are useful for potential applications in nanoelectronics.

A theory of quantum eigenstates of curved and varying cross-sectional waveguides is described by Prof. Morten Willatzen and Dr. Jens Gravesen [5]. A simple one-dimensional differential equation in the centerline coordinate of an arbitrarily curved quantum waveguide with a varying cross section is derived using a combination of differential geometry and perturbation theory. The model can tackle curved quantum waveguides with a cross-sectional shape and dimensions that vary along the axis, which are of immanent importance for modern quantum optics. The present analysis generalizes the previous models that are restricted to either straight waveguides with a varying cross-section or curved waveguides, where the shape and dimensions of the cross section are fixed. The authors carry out 2D wave simulations on a number of complex waveguide geometries and demonstrate an excellent agreement with the eigenstates and energies obtained using their 1D model. The computational benefit in using the present 1D model to calculate both the 2D and 3D wave solutions is significant, and it allows for the fast optimization of complex quantum waveguide design. The derived 1D model illustrates how quantum waveguide eigenstates depend on varying cross-sectional dimensions, the waveguide curvature, and the rotation of the cross-sectional frame. In particular, a gauge transformation reveals that

the individual effects of curvature, thickness variation, and frame rotation correspond to separate terms of geometric potential only. The generalization of the present formalism to electromagnetics and acoustics, accounting appropriately for the relevant boundary conditions, is anticipated.

In summary, the present Special Issue “Topology- and Geometry-Controlled Functionalization of Nanostructured Metamaterials” provides a wide panorama of advanced nanostructured materials, in which topology and geometry efficiently control their functional properties for diverse applications. It is highly motivating to the readers of *Applied Sciences*.

Conflicts of Interest: The authors declare no conflict of interest.

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