



Feature issue introduction: advanced computational nanophotonics: from materials to devices

ALEXANDER V. KILDISHEV,^{1,*} JUEJUN HU,² OLIVIER J.F. MARTIN,³ AND DOUGLAS H. WERNER⁴

¹*Birck Nanotechnology Center, School of Electrical & Computer Engineering, Purdue University, West Lafayette, Indiana 47907, USA*

²*Department of Materials Science & Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*

³*Nanophotonics & Metrology Laboratory, Swiss Federal Institute of Technology Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

⁴*The Pennsylvania State University, Department of Electrical Engineering, University Park, PA 16802, USA*

*kildishev@purdue.edu

Abstract: Computational nanophotonics has already made a disruptive impact on the photonic and optoelectronic industries and has dramatically influenced the ways today's optical engineers create, optimize, and use innovative materials and computer-aided services. This Feature Issue presents a set of eleven papers combined under the joint title of Advanced Computational Nanophotonics: From Materials to Devices. The science and art of computational photonics have a long established history, yet interest in new approaches to advanced multiphysics modeling at the nanoscale and hence to innovatory multi-objective optimization techniques for nanophotonics have been growing exponentially in the last decade, and are now the subject of intense cross-disciplinary research efforts. The papers selected for the Feature Issue present a diverse palette of topics that, for example, include a comprehensive review of new optimization techniques, a fundamental theoretical concept of photonic Dirac monopoles, along with new multiphysics approaches to full-wave material modeling in non-linear nanophotonics and, in particular, to innovative modeling of photonic neural networks. Applications of advanced computational methods are additionally showcased with space-time light control by dynamic metasurfaces, polarization control with structured color all-dielectric metafilms, and an optofluidic system driven by a thermoplasmonic element.

© 2019 Optical Society of America under the terms of the [OSA Open Access Publishing Agreement](#)

1. Introduction

Computational nanophotonics is one of the central tools of the science of light and photonic device engineering. It plays a crucial role in enabling optical technologies ranging from bio-sensing to quantum information processing. Up to the present, a plethora of techniques and commercial software founded on conventional computational electromagnetics methods have been developed. In the past decade, exceptional interest has been growing in the optical science and engineering communities in efficient topological and shape optimization techniques because of their ultimate importance in shortening the design cycle and offering innovative solutions not attainable otherwise. The special focus of this Feature Issue is also put on new approaches built on a multiphysics computational environment that enables tighter integration between different phenomena involved in light-matter interactions and offers a broader range of new modeling opportunities. The Feature Issue presents eleven papers [1–11] that fit a joint theme of Advanced Computational Nanophotonics: From Materials to Devices. The science and art of computational photonics have a long history, yet in the last

decade interest in new approaches to advanced multiphysics modeling at the nanoscale and innovative multi-objective optimization techniques for nanophotonics have been growing exponentially and are now the subject of intense cross-disciplinary research efforts.

2. Summary of papers in the feature issue

This special issue deals with a gamut of recent research starting from artificial and non-linear materials and is inspired by ways in which these multiscale and multiphysics materials can be used to design novel, transformative devices and systems. We open by noting that there has been an exceptional amount of interest in robust methodologies for highly-efficient design optimization because of their ultimate importance in shortening the design cycle as well as their ability to offer innovative solutions not attainable otherwise. Hence, it comes as no surprise that our issue presents three papers dealing with various aspects of optimization techniques [1–3]. In [1], Campbell et al., give a brief review of the most popular techniques, and then provide a detailed discussion of the most recent innovative methods such as topology optimization (TO) and multi-objective optimization. This comprehensive review targeting a broad audience (selected as an Editor's Pick) also includes a discussion of future directions with approaches built on surrogate-modeling and deep learning. A related more specific study [2] indicates that topology-optimized metasurfaces can be made insensitive to shape imperfections by integrating the performance of eroded and dilated shapes into the iterative optimization algorithm. The authors also use the TO refining of conventional designs to make them more robust. Analyzing the robust devices, the authors show that robustness is enforced through rather non-intuitive interactions between excited robust modes and may not be attained with simple design rules [2]. Genevet et al. discuss a computational approach to enable robust metasurface designs by quantifying the impact of fabrication errors on the experimentally fabricated devices [3]. The approach can be useful in designing novel passive and active metasurface components where fabrication deviations often pose a challenge and need to be properly accounted for in the design phase.

Although almost a quarter of the papers in the Feature Issue addresses the use of optimization techniques in nanophotonic or optoelectronic design, advanced numerical multiphysics methods are also intensively used to model non-linear materials and achieve novel desired functionalities, as discussed for example in [4,5]. In their study Varin et al. ([4], an Editor's Pick) show that a set of multiple nonlinear Lorentz oscillator models can be employed to accurately describe nonlinear optical dispersion. The authors derive the non-linear material models from the quantum mechanical two-level atom model with the adiabatic-following, under-resonant approximation and provide a comprehensive analysis of the limits when the proposed framework could be used for modeling nonlinear dispersion of arbitrary complexity. A related effort deals with implementations of activation functions for photonic neurons that dominate current efforts. Hardware implementations of activation functions are of critical importance for neural network connections, learning algorithms, and computational dataflow schemes. In [5] (which is selected for Spotlight on Optics), Miscuglio et al. explore novel concepts of all-optical activation functions: (i) the Fano resonance of a quantum dot coupled with a plasmonic nano-antenna, and (ii) the reverse saturable absorption of a Buckyball-doped polymer film. Based on a full-scale network simulation the authors demonstrate that the hardware realizations of these nonlinear all-optical activation functions are compatible with modern integrated photonics and sufficiently fast to compete with state-of-the-art alternative schemes.

The area of computational nanophotonics also incorporates nascent theoretical developments including topological photonics and quantum information processing. In [6], Van Mechelen et al. introduce the concept of a photonic Dirac monopole that is suitable for the field of spin photonics, topological photonic crystals and metamaterials. Using a Dirac-Maxwell correspondence in the Riemann-Silberstein basis, they further show that the magnetic monopole charge quantization in momentum space arises solely from spin-1

properties of the photon. These topologically massive photons are interpreted as spin-1 skyrmion that arise from nonlocal Hall conductivity.

Advanced methods of computational nanophotonics can also be applied to explore a new reconfigurable environment for light, as shown in this issue with a couple of invited papers [7,8]. In [7], Mosallaei et al., present a fast and accurate numerical technique to compute light propagation through patterned layers with spatial and temporal modulation of permittivity by extending the rigorous coupled-wave analysis framework. They expand the electric and magnetic field components of an arbitrarily shaped space-time unit cell into a basis of spatiotemporal harmonics and compute their modal field profiles as a set of eigenmodes of the unit cell. Unique applications for time modulated metasurfaces based on electro-optical modulation of materials such as silicon and graphene are studied.

In [8], Evlyukhin et al. apply a multipole decomposition method to study the resonant optical responses from cylindrical Si nanodisks illuminated by evanescent light waves in a total internal reflection configuration. The authors demonstrate that the color of the scattered light can be efficiently tuned by rotating the polarization of incident light that generates the evanescent waves. As expected in this case, the omnipotent multipole analysis clarifies the physics of the color formation and offers new non-trivial solutions to various applications, e.g., advanced sensing, quantum communications, and high-resolution color displays.

While the bulk of the papers in the Feature Issue describes the details of new computational techniques and innovative theoretical concepts, the use of the finite-element method (FEM) for specific bio-sensing applications is discussed in two sensing device papers [9,10]. In [9], the authors employ a FEM analysis of a cross-shape nanoantenna for enhancing the emission intensity of an arbitrarily oriented quantum emitter and preserving its orientation information in the far field. In contrast to the previous paper, in [10], the authors perform a numerical study of a novel design of a refractive index sensor. The authors show that their design based on a microfiber coated with gold nanowires improves the performance of the sensor by about 40% in comparison with the microfiber coated with a gold film.

The Feature Issue concludes with an exciting application of numerical coupling of multiple physics in a single problem. In [11] Hong et al. combined optics, thermodynamics, and hydrodynamics in a multiphysics finite element framework to simulate the temperature rise resulting from the photothermal heating of a plasmonic TiN bowtie nanoantenna and the associated hydrodynamic flow generated in a microfluidic channel. The authors demonstrate that the electrothermoplasmonic flow velocity induced by the TiN nanoantenna is more than three times higher vs. that of a gold nanoantenna. This prediction makes TiN a plasmonic material of choice in microfluidic devices with optically-controlled heat, fluidic dynamics, and heat-induced forces. We note that although all of the last three studies [9–11] use a commercial FEM solver (Comsol Multiphysics), only [11] employs advanced coupling of multiple physics in overlapping simulation domains.

To summarize, we truly believe that the representative collection of review and research papers on current and future trends in computational nanophotonics presented here will assist the larger community of photonics as well as optical material science in understanding transformative developments and acquiring new ideas in optical device optimization and computer-aided design.

Acknowledgments

The editors are grateful to all the authors who contributed their review and research papers to our Feature Issue. We also want to thank all the reviewers for taking the time to share with us their constructive feedback and comment on the submissions in a timely fashion. Our special thanks to the Optical Materials Express editorial staff who supported and guided us through the entire process from planning the submissions to reviewing and virtual publishing.

References

1. S. D. Campbell, D. Sell, R. P. Jenkins, E. B. Whiting, J. A. Fan, and D. H. Werner, "Review of numerical optimization techniques for meta-device design[Invited]," *Opt. Mater. Express* **9**(4), 1842–1863 (2019).
2. E. W. Wang, D. Sell, T. Phan, and J. A. Fan, "Robust design of topology-optimized metasurfaces," *Opt. Mater. Express* **9**(2), 469–482 (2019).
3. N. Schmitt, N. Georg, G. Brière, D. Loukrezis, S. Héron, S. Lanteri, C. Klitis, M. Sorel, U. Römer, H. De Gersem, S. Vézian, and P. Genevet, "Optimization and uncertainty quantification of gradient index metasurfaces [Invited]," *Opt. Mater. Express* **9**(2), 892–910 (2019).
4. C. Varin, G. Bart, T. Fennel, and T. Brabec, "Nonlinear Lorentz model for the description of nonlinear optical dispersion in nanophotonics simulations [Invited]," *Opt. Mater. Express* **9**(2), 771–778 (2019).
5. M. Miscuglio, A. Mehrabian, Z. Hu, S. I. Azzam, J. George, A. V. Kildishev, M. Pelton, and V. J. Sorger, "All-optical nonlinear activation function for photonic neural networks [Invited]," *Opt. Mater. Express* **8**(12), 3851–3863 (2018).
6. T. Van Mechelen and Z. Jacob, "Photonic Dirac monopoles and skyrmions: spin-1 quantization [Invited]," *Opt. Mater. Express* **9**(1), 95–111 (2019).
7. S. Inampudi, M. M. Salary, S. Jafar-Zanjani, and H. Mosallaei, "Rigorous space-time coupled-wave analysis for patterned surfaces with temporal permittivity modulation [Invited]," *Opt. Mater. Express* **9**(1), 162–182 (2019).
8. A. B. Evlyukhin and S. I. Bozhevolnyi, "Polarization control of colors in resonant evanescent field scattering by silicon nanodisks [Invited]," *Opt. Mater. Express* **9**(1), 151–161 (2019).
9. L. Ma, S. Sun, T. Zhang, R. Li, Q. Du, J. Zhang, and M. Li, "Highly-symmetrical plasmonic nanoantenna for fluorescence enhancement and polarization preservation of arbitrarily oriented fluorophore," *Opt. Mater. Express* **8**(12), 3770–3786 (2018).
10. Y. Zhan, Y. Li, Z. Wu, S. Hu, Z. Li, X. Liu, J. Yu, Y. Huang, G. Jing, H. Lu, H. Guan, W. Qiu, J. Dong, W. Zhu, J. Tang, Y. Luo, J. Zhang, and Z. Chen, "Surface plasmon resonance-based microfiber sensor with enhanced sensitivity by gold nanowires," *Opt. Mater. Express* **8**(12), 3927–3940 (2018).
11. C. Hong, S. Yang, and J. C. Ndukaife, "Optofluidic control using plasmonic TiN bowtie nanoantenna [Invited]," *Opt. Mater. Express* **9**(3), 953–964 (2019).