Research Statement

Data Center Hardware Based on Nanomaterials
– *Bringing the Power of Nanoscale to the Macroscopic World* –

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Overview

One of the grand challenges in nanoengineering and nanoscience today is how to create macroscopic materials and devices by assembling nano-objects *while preserving their rich variety of extraordinary properties* that are promising for new applications. My research program will address this long-standing problem in the context of data center hardware. Because of the rapidly increasing volume of datasets, there is a strong demand for enhancing the capability and energy efficiency of data centers. The extraordinary electronic, optical, and thermal properties of nanomaterials can offer unprecedented tools for performing heat management, maximizing bandwidth, and boosting energy efficiency. Through my doctoral and postdoctoral research, I have acquired deep and extensive knowledge of the physical properties of a variety of nanomaterials, as well as strong expertise in assembling them into ordered macroscopic architectures. The overall goal of my multidisciplinary research program will be to unleash unprecedented modern nanomaterial properties to the macroscopic world for solving two of the main challenges we are facing in this information age: (1) How can data be transmitted and processed quickly and efficiently given limited resources?, and (2) How can we produce more sustainable resources for powering these devices?

Previous Accomplishments

My doctoral and postdoctoral research has focused on the development of photonic and optoelectronic devices that operate in the terahertz (THz), midinfrared (MIR), and near-infrared (NIR) ranges using graphene and single-wall carbon nanotubes (SWCNTs).

Graphene optoelectronics: Graphene is promising for developing high-speed modulators [1], but their performance remained low due to its poor ability to absorb light. I overcame this challenge by combining graphene with nanophotonic structures, including THz extraordinary-optical-transmission (EOT) metamaterials [2], MIR guided-mode resonance [3, 4], and NIR dielectric microring resonators [5] (Fig. 1a). These hybrid architectures enhanced light-matter interaction in graphene for efficient electro-optic modulation, which are also CMOS-compatible for industrialization.

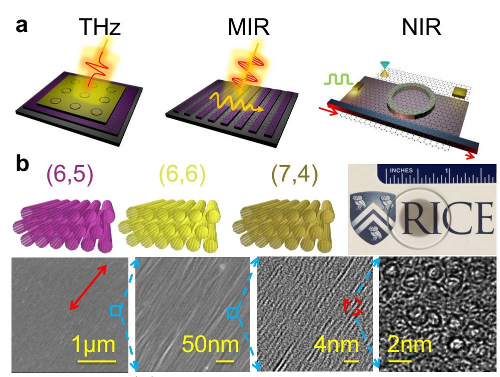

Figure 1: (a) Graphene THz, MIR, and NIR devices. (b) Wafer-scale crystalline SWCNTs.

Wafer-scale crystalline single-chirality SWCNTs: Individual SWCNTs exhibit extraordinary anisotropic electronic, optical, thermal, and mechanical properties, but the macroscopic manifestation of such properties has been limited due to polydispersity and randomness in ensemble assemblies. I have made a breakthrough toward the *holy grail* of fabricating wafer-scale crystalline films of single-chirality SWCNTs, through a low-cost self-assembly vacuum filtration process. I successfully fabricated large-area (2 inch) monodomain films of aligned SWCNTs [6, 7], with perfect alignment, ultrahigh packing density $\sim 10^6/\mu\text{m}^2$, and controllable thickness from a few nanometers to microns (Fig. 1b). Obtained films can be micro/nano-manufactured to create 3D architectures by intercalating molecules and stacking multiple layers [7]. This technique is expected to be universally applicable to any high aspect-ratio nanostructures. This discovery immediately opens up exciting new opportunities. For example, I have observed microcavity exciton-polaritons by embedding aligned (6,5) SWCNTs inside a photonic cavity. This novel quantum optical structure displayed a record-breaking value of vacuum Rabi splitting (VRS ~ 329 meV), on-demand ultrastrong coupling through polarization control, and exceptional points in dispersions, promising for novel quantum technology [8]. Furthermore, I demonstrated that these aligned SWCNT films make an ideal refractory nanophotonic platform for waste heat recovery, because of their ultrastable tubular structure and extreme anisotropy [9].

Future Research

My future research as a faculty member will focus on data center hardware based on nanomaterials. I will reveal the extraordinary electronic and optoelectronic properties of nanomaterials on a macroscopic scale to upgrade and revolutionize hardware for efficient networking, high-performance computing, and sustainable powering. My *nanomaterial library* includes wafer-scale crystalline nanotubes that are *exclusively available* through my vacuum filtration technique, graphene, and extends to phase change materials (PCMs) and transition metal dichalcogenides (TMDs). By fully utilizing my uniquely multidisciplinary expertise in materials science, physics, and electrical and computer engineering, I will develop scalable strategies to transmit and process big data with ultrahigh speeds and energy efficiency. Specifically, my research program will consist of the following three thrusts:

THRUST 1: EFFICIENT DATA CENTER NETWORKING

Emerging THz wireless links offer ultrabroad bandwidth for terabit-per-second data speeds. Essential THz components, such as modulators and sources, are still underdeveloped. In this thrust, I will employ nanomaterials to improve their performance.

Ultrafast, low-power, nonvolatile, reconfigurable THz modulators: Reconfigurable metamaterials are great candidates for THz modulators, however, current devices are slow, volatile, and require high operation power. I will address these challenges by incorporating nonvolatile PCMs in EOT metamaterials (Fig. 2a). PCMs introduce a fast (gigahertz) and drastic optical conductivity change, and thus a strong modulation depth $> 20\,\mathrm{dB}$, during a phase transition under external stimulus. Small PCM pieces in the current path of metamaterials and unique aligned CNT electrodes can solve the challenges of large-area nonuniformity and high excitation power of PCMs, with a low-power consumption $\sim$100 fJ/bit [10].

Nonlinear optical (NLO) materials for THz sources: Optical nonlinearity is the key for THz wave generation. NLO materials with large $\chi^{(2)}$ and low thresholds are strongly desirable for continuous-wave on-chip operation. I will investigate the NLO properties of aligned SWCNTs encapsulating molecules. Nanoconfined 1D space in hollow SWCNTs provides an ideal head-to-tail alignment of NLO molecules [11] instead of antiparallel dipole arrangement in the bulk. I will deploy the vacuum filtration technique for producing crystalline SWCNTs encapsulating molecules, such as p,p-dimethylaminonitrostilbene with hyperpolarizability $\sim 7 \times 10^{-26}$ e.s.u., which render giant $\chi^{(2)} \sim 600\,\mathrm{pm/V}$ in the NIR (Fig. 2b). The developed materials can form thin films for easy phase matching, and can be readily combined with resonators to further reduce the power threshold for integrated THz sources.

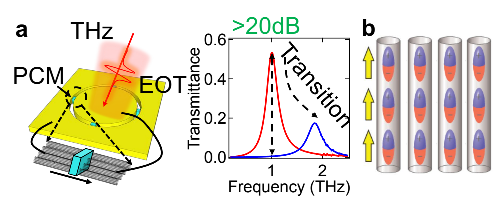

Figure 2: (a) THz modulators based on PCMs. (b) NLO aligned encapsulated SWCNTs.

THRUST 2: ADVANCED DATA CENTER COMPUTING

Brain-inspired and quantum-mechanics-inspired architectures are two emerging mainstream pathways toward the next-generation high-performance computing hardware. In this thrust, I will implement these functionalities using photonic structures based on carbon nanomaterials.

<u>*Photonic artificial neural networks (ANNs)*</u>: Due to their inherent parallelism, ultrabroad bandwidth, and passive operation, photon-based non-Von Neumann architectures are promising for handling large datasets. Activation functions (red dots in Fig. 3a) mimicking our brains perform nonlinear operations in general ANNs, and saturable absorbers are promising candidates for photonic implementation. For example, their general response resembles the popular Leaky ReLU activation function (Fig. 3b). Among various saturable absorbers, graphene is theoretically predicted to possess a surprisingly low power threshold for continuous-wave operation [12], and its electrical tunability is ideal for training processes. I will integrate graphene in an optical waveguide, demonstrate electrically controllable nonlinearity under continuous-wave excitation, and build chips performing specific tasks such as pattern recognition utilizing machine learning algorithms.

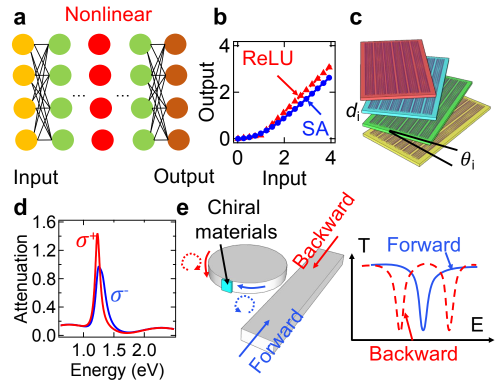

Figure 3: (a) A general model of ANNs. (b) Saturable absorber and Leaky ReLU responses. (c) Twisted stacks of aligned SWCNTs and (d) their response. (e) Chiral light-matter interactions.

<u>*Chiral quantum optics interfaces*</u>: Chiral light-matter interaction provides an exciting new element in building fundamental components and controlling information flow for quantum computation. It is crucial for practical applications to develop room-temperature chiral materials, possessing circular-polarization-dependent dipole transitions without external stimulus. Existing natural chiral molecules have very weak optical activity with ellipticity per thickness $< 10^{-2}$ deg/μm. SWCNT enantiomers, in contrast, show strong *intrinsic* optical activity around excitonic transitions [13]. I will first create crystalline SWCNT enantiomers using the vacuum filtration method, which render giant optical activity $\sim$25 deg/μm. Furthermore, I will create macroscopic *extrinsic* chiral materials by stacking films of aligned SWCNTs without enantiomer separation in a chiral manner. I will have a precise control of rotation angles, θ_i, and thicknesses, d_i, using my developed stacking technique (Fig. 3c). A 250-nm thick macroscopic film can demonstrate strong circular-polarization-dependent absorption (Fig. 3d). This twisted stacking strategy can apply to other materials such as graphene and TMDs. On the other hand, optical chirality emerges naturally in nanophotonic structures, where transverse optical confinement leads to propagation-direction(k)-dependent ellipticity of the evanescent field, known as spin-momentum locking. I will integrate these materials with resonators for k-dependent strong coupling (Fig. 3e).

THRUST 3: SUSTAINABLE DATA CENTER POWERING

Recycling the waste heat and mechanical vibration generated from data centers will increase both power and cost efficiencies. In this thrust, I will build sustainable generators by harvesting heat and mechanical energy using wafer-scale crystalline 1D nanotubes.

<u>*Waste heat harvesting*</u>: Crystalline SWCNTs will lead to the development of transformational thermophotovoltaics and thermoelectrics for building efficient heat-to-electricity converters. I propose a novel high-efficiency near-field thermophotovoltaic (NFTPV) cell by incorporating two parallel films of mechanically strong, hyperbolic, aligned p-doped SWCNTs separated by a vacuum gap (Fig. 4a). The near-field coupling of high-k waves can boost the near-field (far-field) heat transfer by at least one order (two orders) magnitude [14] due to an enhanced photonic density of states (DOS). On the other hand, an enhanced electronic DOS in SWCNTs can boost the thermoelectric figure-of-merit ZT factor, which depends on the Seebeck coefficient (S), electrical and thermal conductivity (σ and κ) through $ZT \propto S^2\sigma/\kappa$. However, it is unclear how film morphology and carrier

density affect the ZT factor. My developed macroscopic crystalline SWCNTs are compatible with various dopants and measurement techniques, ideal for detailed investigation. In addition, I will use vacuum filtration to align encapsulated SWCNTs (Fig. 4b) for reducing κ.

Mechanical motion harvesting: Piezoelectrics form the core components of these harvesters. Conventional ceramics are strong piezoelectrics but are brittle, heavy, and toxic. Flexible polymers are usually weak piezoelectrics. Boron nitride nanotubes (BNNTs) have high mechanical strength, low environmental impact, and display an excellent piezoelectric response when they are aligned. I will develop recipes of aligning BNNTs using vacuum filtration, study piezoelectric properties, and build real devices (Fig. 4c).

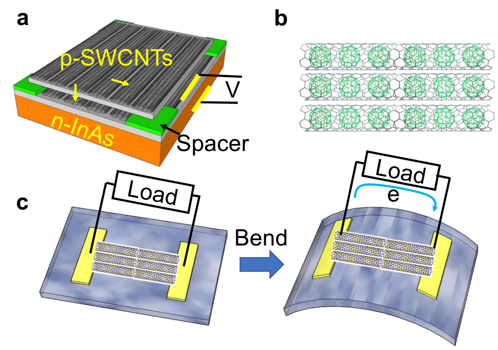

Figure 4: (a) NFTPV cells. (b) Aligned encapsulated SWCNTs. (c) Piezoelectricity in aligned BNNTs.

Collaboration

There will also be diverse collaboration opportunities with colleagues across campus. In collaboration with Dr. Zhaoyang Fan from Nano Tech center, we will investigate to build THz optoelectronic devices based on nanomaterials. For example, we will study coherent plasmon resonance in nanopatterned films of crystalline SWCNTs, originating from bounded charge oscillations by nanotube ends. This resonance is broadly tunable in the THz range through the adjustment of pattern geometry and free-carrier concentration, enabling applications of THz modulators and detectors.

From a multidisciplinary perspective, atomically smooth inner walls of crystalline (6,6) SWCNTs produced using vacuum filtration increase water permeability by five orders of magnitude and can fully reject salts, ideal for water desalination; strong coupling between semiconducting SWCNTs and gold nanoparticles attached on the sidewall makes the lowest energy state become the bright lower polaritons instead of dark excitons, enhancing efficiency for deep-tissue NIR fluorescence imaging; large-area, highly conductive, flexible electrodes made of SWCNTs are advantageous over stiff counterparts for neural recording.

1. Gao, W. *et al. Proc. SPIE* **8984,** 89840K (2014).
2. Gao, W. *et al. Nano Lett.* **14,** 1242 (2014).
3. Gao, W. *et al. ACS Nano* **6,** 7806–7813 (2012).
4. Gao, W. *et al. Nano Lett.* **13,** 3698–3702 (2013).
5. Qiu, C. *et al. Nano Lett.* **14,** 6811–6815 (2014).
6. He, X. *et al. Nat. Nanotechnol.* **11,** 633–638 (2016).
7. Komatsu, N. *et al. Adv. Funct. Mater.* **27,** 1606022 (2017).
8. Gao, W. *et al. Nat. Photonics* **12,** 362–367 (2018).
9. Gao, W. *et al. under review.*
10. Xiong, F. *et al. Science* **332,** 568–570 (2011).
11. Cambré, S. *et al. Nat. Nanotechnol.* **10,** 248–252 (2015).
12. Marini, A. *et al. Phys. Rev. B* **95,** 125408 (2017).
13. Wei, X. *et al. Nat. Commun.* **7,** 12899 (2016).
14. Liu, X. *et al. Appl. Phys. Lett.* **103,** 213102 (2013).