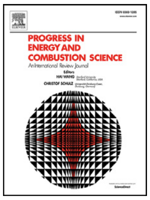
Progress in Energy and Combustion Science 000 (2017) 1–35

Contents lists available at ScienceDirect

Progress in Energy and Combustion Science

journal homepage: www.elsevier.com/locate/pecs



# Carbon nanotubes: A potential material for energy conversion and storage

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ARTICLE INFO

*Article History:*
Received 13 July 2017
Accepted 24 October 2017
Available online xxx

ABSTRACT

Carbon nanotube-based materials are gaining considerable attention as novel materials for renewable energy conversion and storage. The novel optoelectronic properties of CNTs (e.g., exceptionally high surface area, thermal conductivity, electron mobility, and mechanical strength) can be advantageous for applications toward energy conversion and storage. Although many nanomaterials are well known for the unique structure-property relations, such relations have been sought most intensively from CNTs due to their extreme diversity and richness in structures. For the development of energy-related devices (like photovoltaic cells, supercapacitors, and lithium ion batteries), it is critical to conduct pre-evaluation of their design, operation, and performance in terms of cost, life time, performance, and environmental impact. This critical review was organized to address the recent developments in the use of CNT-based materials as working/counter electrodes and electrolytes in photovoltaic devices and as building blocks in next-generation flexible energy storage devices. The most promising research in the applications of CNTs toward energy conversion and storage is highlighted based on both computational and experimental studies along with the challenges for developing breakthrough products.

## Contents

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*Abbreviations:* CAGR, Compound annual growth rate; CNF, Carbon nanofiber; CNTs, Carbon nanotubes; CSA, Chlorosulfonic superacid; CVD, Chemical vapor deposition; D3PIE, Dynamic three-phase interline electropolymerization; DFT, Density functional theory; DSSCs, Dye-sensitized solar cells; DWCNTs, Double-walled carbon nanotubes; EDLC, Electrical double layer capacitor; FT, Filtration-transfer; FTO, Fluorine-doped tin oxide; GNS, Graphene nanosheet; GO, Graphene oxide; HiPCO, High-pressure carbon monoxide; ICP, Intrinsically-conducting polymers; IPCE, Incident photon-to-charge conversion efficiency; ITO, Indium-doped tin oxide; LB, Langmuir-Blodgett; LCD, Liquid crystal display; LD, Local density; LIBs, Lithium-ion batteries; MC, Monte Carlo; MD, Molecular dynamics; $MeO_x$, Metal oxide; $MoO_x$, Molybdenum oxide; m-MWCNTs, Metallic multi-walled carbon nanotubes; MWCNTs, Multi-walled carbon nanotubes; N-CNTs, Nitrogen-doped carbon nanotubes; OLEDs, Organic light emitting devices; OMC, Organic-modified clay; oMWCNTs, Carboxylic group-functionalized MWCNTs; OPVs, Organic photovoltaic cells; OER, Oxygen evolution reaction; ORR, Oxygen reduction reaction; PAN, Polyacrylonitrile; PAni, Polyaniline; PCE, Power conversion efficiency; PEDOT:PSS, Poly(3,4-ethylenedioxythiophene):poly- (styrenesulfonate); PET, Polyethylene terephthalate; PMII, 1-methyl-3-propylimidazolium iodide; PMMA, Poly(methyl methacrylate); POEM, Poly(oxyethylene)-segmented oligo(amide-imide); PPImI, 1-propyl-3-methylimidazolium iodide; PPy, Polypyrrole; PV, Photovoltaic; RGO, Reduced-graphene oxide; RGONR, Reduced-graphene oxide nanoribbon; SACNTs, Super-aligned carbon nanotubes; S-a-PCNT, Sulfur-immobilized activated porous CNT; SWCNTs, Single-walled carbon nanotubes; s-SWCNTs, Semiconducting single-walled carbon nanotubes; TBA, Tetrabutyl ammonium; TBMD, Tight binding molecular dynamics; TCEs, Transparent conducting electrodes; TCFs, Transparent conducting films; TCO, Transparent conducting oxide; TMC, Transition metal compound; VASWCNTs, Vertically-aligned single-walled carbon nanotubes

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http://dx.doi.org/10.1016/j.pecs.2017.10.005

Please cite this article as: S. Kumar et al., Carbon nanotubes: A potential material for energy conversion and storage, Progress in Energy and Combustion Science (2017), http://dx.doi.org/10.1016/j.pecs.2017.10.005

## 1. Introduction

The exponentially increasing demand for renewable energy, accompanied by the rise of high-speed, portable, wearable, and transparent electronic devices, has sped up the development of new techniques not only to catch up such unprecedented challenges but also to produce new device architectures. A promising solution for such challenges lies in nanotechnology of which advent can help stimulate the invention and fabrication of many advanced materials with innovative performance. The material structure can be tunable by nanotechnology which endowed nanomaterials with highly unique and novel properties and new opportunities in various fields of applications (e.g., energy conversion and storage, water treatment, contaminant sensing, and molecular biology).

Nanomaterials have been widely investigated as electrodes and electrolytes in energy conversion and storage applications due to their many advantageous properties. In particular, carbon-based nanomaterials (e.g., 2D graphene sheets, 1D carbon nanotubes, and 0D fullerenes) have drawn particular attention due to their properties, which are derived from their atomic structure and surface chemistry. Among the wide variety of nanomaterials, carbon nanotubes (CNTs) possess one of the unique nanostructures due to their fine chemical composition and atomic-bonding configuration. Additionally, CNTs possess strong structure-property relations based on highly diverse structures [1]. The electro-mechanical properties of CNTs have been investigated intensively since their finding in early 1990s. Although early research centered on their growth and characterization, the focus shifted toward diverse commercial fields ranging from photovoltaic (PV) to sensing applications (e.g., by integrating them into thin-film electronics) [2–8]. As we will demonstrate in this review, there have been growing interests in using CNTs in a range of applications.

Because of their many fascinating properties (e.g., good mechanical strength and elasticity, high electronic sensitivity to mechanical strain and chemical absorbates, good electronic properties ranging from semiconductor to metals, and very large surface area-to-volume ratio), the use of CNTs has been recommended for diverse applications such as components of PV devices, energy storage devices, chemical sensors, actuators, and metrology-probe tips [9–12]. In this review, we focused on the role of CNT-based materials in energy conversion and storage. Existing studies directed to both theoretical and computational aspects of CNTs are all discussed. We also detailed the challenges associated with their practical application toward commercialization.

## 2. Carbon nanotubes: concepts and properties

CNTs with their unique morphologies and novel physicochemical properties, represent promising materials for future applications. They are one-dimensional allotropes of carbon where hexagonally-oriented carbon atoms have a cylindrical nanostructure. Carbon-based nanomaterials are classified depending on their atomic bonding (*sp*, $sp^2$, and $sp^3$ hybridizations) and dimensionality [13]. Globally, the commercial interest in CNTs has been reflected in their production capacity which is estimated to exceed several thousand tons per year while growing continuously [14]. The CNT mass production is a multi-level process that includes molecules, material, reactor, process, and system level engineering, as shown in Fig. 1 [15]. The molecular level engineering is based on the formation of CNTs via chemical route. It concerns on the tunable structure of CNTs, e.g., crystallinity, wall number, defect, length, and chirality with the help of such variables as proper growth windows, use of proper catalysts, and carbon sources. The production cost of CNTs can be estimated easily with the help of selected chemical route and operating window. The material-level engineering emphasizes the strong interactions among CNTs that can lead to several types of agglomerates including aligned CNTs, entangled CNTs, and sparse CNTs. It requires a better knowledge of CNTs with respect to their structure, position, alignment, and quality control. Further, the third-level engineering is related to the domain of CNTs production with consideration of their hydrodynamics, apparent/intrinsic kinetics, heat/mass transfer kinetics, and catalyst deactivation. The forth-level process engineering relies on the construction of facilities required for continuous and mass production of CNTs, e.g., purification, automation, packaging, and delivery. There are several factors that can help in improving the efficiency of the system such as: (i) molecular scale intensification, (ii) saving of feedstock, and (iii) multi-functionality of the reactor. The last level of the CNT mass production is related to environmental as well as ecological considerations about their production and commercial applications. It should thus consider the effect of CNTs exposure on human health and biosphere.

Further, several synthesis strategies for CNTs have been developed, e.g., arc discharge [16], chemical vapor deposition (CVD) [17], laser ablation [18], electrolysis [19], pyrolysis [20], flame synthesis [21], electron or ion beam irradiation [22], and solar approaches [23]. The laser ablation and arc discharge of graphite are common techniques for production of CNTs from carbon vapor. These CNTs can maintain good quality with a fewer structural defects due to the

Please cite this article as: S. Kumar et al., Carbon nanotubes: A potential material for energy conversion and storage, Progress in Energy and Combustion Science (2017), http://dx.doi.org/10.1016/j.pecs.2017.10.005