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Frontiers of Advanced Sciences and Technologies: Results, Challenges and Perspectives

Hongbo Gu,[1,*] Zhanhu Guo,[2] Nithesh Naik,[3] Dasharathraj K Shetty,[4] BM Zeeshan Hameed,[5] Udit Kumar Chakraborty,[6] Rahul Paul,[7] Manjunath K Vanahalli,[8] Devesh Kumar Srivastava,[9] Anish Gupta,[10] Babita Singla,[11] Sarvesh Kumar,[12] Nishu Aaydee,[13] Chuntai Liu,[14] Qing Hao,[15] Hang Zhang,[16] Santosh Patil,[17] Bibin John,[18] Saravanan Karuppanan,[19] Luyi Sun,[20] Tuan Quoc Le,[21] Baskar Gurunathan,[22] Chandrasekaran Muthukumaran,[23] Sham Aan M.P,[24] Na Lu,[25] Hongyu Nick Zhou,[26] A.N.Manoharan[27] and Balakrishna Maddodi[28]

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Engineered Science could facilitate the connection of scientists and engineers from academia and industries. A better understanding and interpretation of the science, engineering and technology can dramatically advance the development of our society and benefit our everyday lives. This special issue aims to provide the frontier scientific works from both inter- and intra-disciplines such as artificial intelligence (AI) and machine learning (ML), healthcare, and discovery of new materials for important applications.

AI, as an intelligence demonstrated by machines to imitate the natural intelligence owned by humans and animals, has shown promising perspectives in materials science and engineering.[1] As one subfield of AL, ML has become one central topic for materials research and other field.[2] In the ML process, the existing knowledge of materials synthesis and operations can be used to train a machine for the predictions of the automated experimental designs, optimization of the desired structures, and special properties at a reasonable level of accuracy. Here the machine learns the information and rules from a large amount of scientific works that is called big data through the statistical algorithms.[3,4] As a result, this could minimize the tremendous efforts to carry out experiments and simulations, and speed up the materials discovery as well as predict future results and trends. As one example in thermal sciences,[5] Fig. 1 describes a cycle for the discovery of thermal-material with the assistant of a ML process. As an early successful high accurate computational method to calculate the thermal conductivity, the advanced methods like ab-initio density functional theory (DFT) and Green-Kubo formulation, *etc*. mainly based on the one directional model and quite expensive. On the contrary, the ML process could efficiently complete the materials discovery cycle by the correlation between thermal conductivity and descriptors (*e.g*., materials descriptors and transport descriptors). Benefiting from this feedback, the thermal-materials innovation and discovery could be significantly speeded up. In addition, ML could also accelerate the research into the new energy systems and electronic devices.[6] On the one hand, ML could be adopted to largely replace quantum simulations to determine the potential chemical molecules and materials for batteries,[7] organic light-emitting diodes (OLED),[8] and carbon dioxide conversion catalysts in the energy fields.[9] On the other hand, it could also help forecast the possible properties of energy systems. For instance, He *et al*.[10] employed the ML to optimize the component size of a hybrid system consisting of

[1] *Shanghai Key Lab of Chemical Assessment and Sustainability, School of Chemical Science and Engineering, Tongji University, Shanghai 200092, China.*
[2] *Integrated Composites Laboratory (ICL), Department of Chemical & Biomolecular Engineering, University of Tennessee, Knoxville, TN, 37996, USA.*
[3] *Department of Mechanical and Manufacturing Engineering, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka 576014, India.*
[4] *Department of Humanities and Management, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka 576104, India.*
[5] *Department of Urology, Father Muller Medical College, Mangalore, Karnataka 575002, India.*
[6] *Department of Computer Science & Engineering, Sikkim Manipal Institute of Technology, Sikkim Manipal University, Sikkim 737136, India.*
[7] *Department of Radiation Oncology, Harvard Medical School, Boston, Massachusetts, USA.*
[8] *Data Science and Intelligent Systems, Indian Institute of Information Technology, Dharwad, India.*

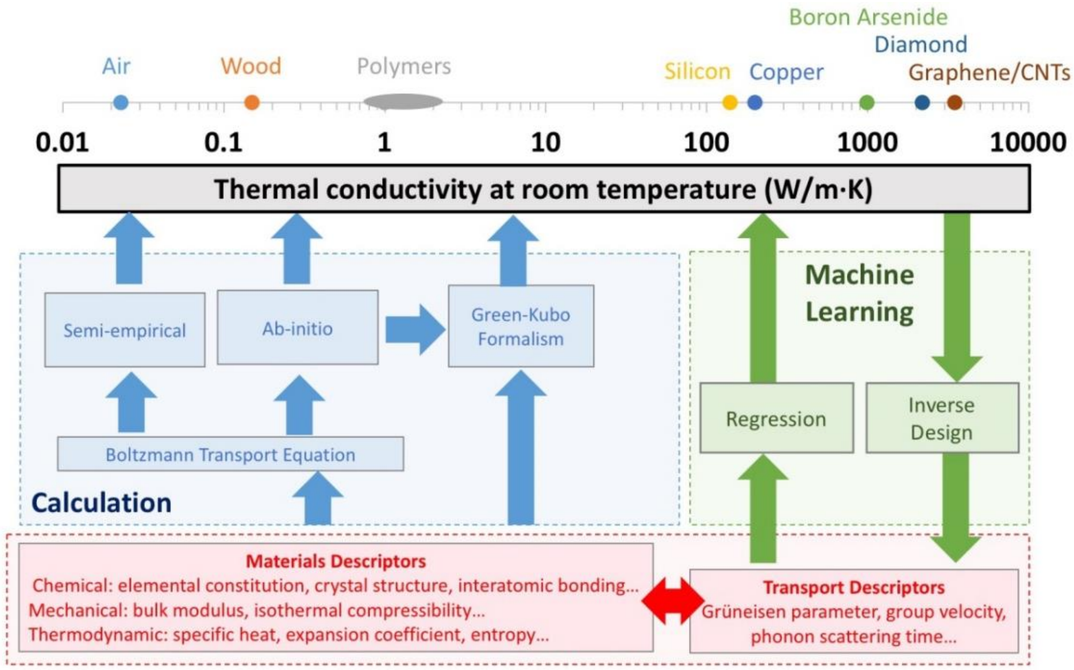

Fig. 1 Standard process in thermal-materials discovery by machine learning and calculations. Reproduced with the permission from [5]. Copyright Engineered Science Publisher LLC 2018.

a photovoltaic (PV) cell and a thermoelectric generator (TEG) and predicted the optimal output power of this photovoltaic thermoelectric hybrid system. This work provided a reference for the structural optimization in the energy fields.

In addition, the materials science and engineering exhibit the essential role in the healthcare field as well. Taking the treatment of liver fibrosis (which is a pathological feature of the chronic hepatic damage and could causes cirrhosis and hepatocellular carcinoma[11]) as an example, Hayashi *et al*.[12] developed an effective approach by the surface engineering of nanoparticles to reverse the liver fibrosis process by the inactivation of the hepatic stellate cells (HSCs), which is one type of cells in the liver and plays an important role in the progress of liver fibrosis by generating the extracellular matrix (ECM) proteins and leading to the chronic liver injury.[13] They reported a novel organic-inorganic (silica) hybrid hollow nanoparticles (HNPs) composed of disulfide and siloxane components and a surface containing thiol groups for targeting delivery of silibinin (SIL) to HSCs. By the surface modification of HNPs with retinol (one type of vitamin A) *via* the reaction with the thiol groups on the surface of HNPs, the retinol-HNPs were delivered to the HSCs through RBP-receptor-mediated endocytosis, and then accompanied with the clearage of disulfides in HNPs into the thiols by the intracellular glutathione, the SIL was released into the cell. With the synergistic interaction of SIL and vitamin A, the

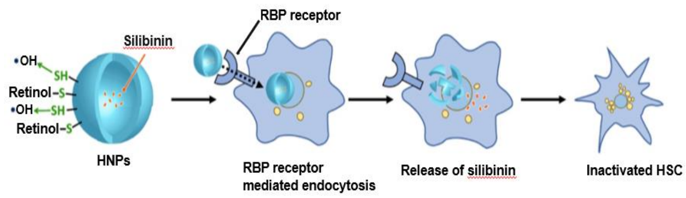

Fig. 2 Schematic illustration of vitamin a grafted organic-inorganic (silica) hybrid hollow nanoparticles (HNPs) for hepatic stellate cells (HSC) targeting delivery. Reproduced with the permission from [11,12]. Copyright Engineered Science Publisher LLC 2019 and WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim 2018.

[9] *Department of Information Technology, Manipal University Jaipur, Rajasthan, India.*
[10] *Apex Institute of Technology, Chandigarh University Mohali, Punjab 752101, India.*
[11] *Chitkara Business School, Chitkara University, Patiala, Chandigarh Tehsil, Rajpura, Punjab 140401, India.*
[12] *Department of Computer Science & Engineering, Babu Banarasi Das University, Lucknow, Uttar Pradesh 226028, India.*
[13] *Bharti Vidyapeeth, Institute of Management and Research, New Delhi 110063, India.*
[14] *Division of Material Science and Engineering, Zhengzhou University Zhengzhou, China.*
[15] *Department of Aerospace and Mechanical Engineering, The University of Arizona, Tucson, AZ, USA.*
[16] *Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing, China.*
[17] *Department of Mechanical Engineering, Manipal University Jaipur, Jaipur, Rajasthan 303007, India.*
[18] *School of Mechanical Engineering, Vellore Institute of Technology, Vellore, Tamil Nadu 632014, India.*
[19] *Mechanical Engineering Department, Universiti Teknologi PETRONAS, 32610 Bandar Seri Iskandar, Perak, Malaysia.*

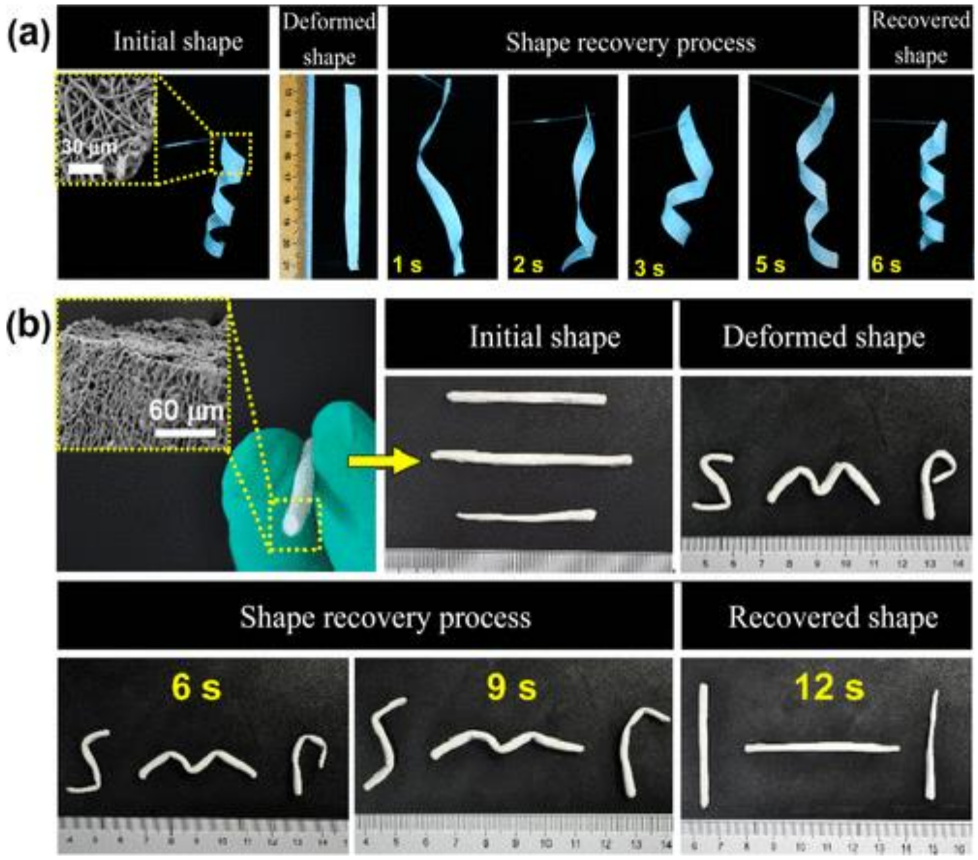

Fig. 3 Illustration on the shape memory effect in the PLMC fibrous scaffolds. (a) Shape recovery process of a membranous form at 39 °C for 6 s; (b) shape recovery process of the cylindrical bars from electrospun fibers at different time of 6, 9, and 12 s at 39 °C as well. Reproduced with the permission from [14,15]. Copyright The Author(s) 2021 and American Chemical Society 2014.

HSCs were inactivated and the tissue was repaired, Fig. 2. Citing another example, shape memory polymers (SMPs), as one type of stimuli-responsive polymers that could obtain a temporary shape and return to its original shape under the stimuli, have gained increasing attention in the medical science and technology, particularly for the development of minimally invasive surgery (MIS).[14] SMPs could transit to the required shape at the desired location once they are implanted in a temporary fixed/compressed position during MIS process, which could totally change the idea of the traditional surgery. Bao *et al*.[15] manufactured an electrospun poly (D,L-lactide-co-trimethylene carbonate) (PLMC) fibrous scaffolds with shape memory properties for the possibility as implants for healing bone screw holes or as barrier membranes for guiding the bone regeneration in the MIS, which exhibited a fast recovery capability within 12 s at 39 °C arising from their excellent shape-changing tailorability for both 2-D (membranous form) or 3-D structures (cylindrical bars), as displayed in Fig. 3.

Especially, the imperative role of materials science and engineering is also reflected in the battle against the virus like severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) disease that was caused by the coronavirus, also named as COVID-19 by the World Health Organization (WHO).[16] For instance, Fig. 4 lays out the typical composition for a medical mask,[17] which is composed of three folded layers of fabrics (two outside layers are spunbonded polypropylene, and the middle layer is melt blown polypropylene) with a loose edge fitting.[18] The main material in the mask is polypropylene, which is melt blown into non-woven fabric and then gets

[20] Department of Chemical & Biomolecular Engineering, Institute of Materials Science, University of Connecticut, USA.
[21] Department of Food Technology, School of Health Science, Hoa Sen University, Thành phố Hồ Chí Minh,, Vietnam.
[22] Department of Biotechnology, St. Joseph's College of Engineering, Chennai, India.
[23] Department of Industrial Biotechnology, Government College of Technology, Coimbatore, India.
[24] Department of Chemistry, R V College of Engineering, Bangalore, Karnataka 560059, India.
[25] Civil Engineering/School of Materials Engineering, Purdue University, West Lafayette, Indiana, USA.
[26] Department of Civil and Environmental Engineering, University of Tennessee, Knoxville, USA.
[27] Department of Post-Graduate Studies and Research in Geology, Government College Kasaragod, Kerala, India.
[28] Department of Civil Engineering, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka 576104, India.
**E-mail:* hongbogu2014@tongji.edu.cn (H. Gu)

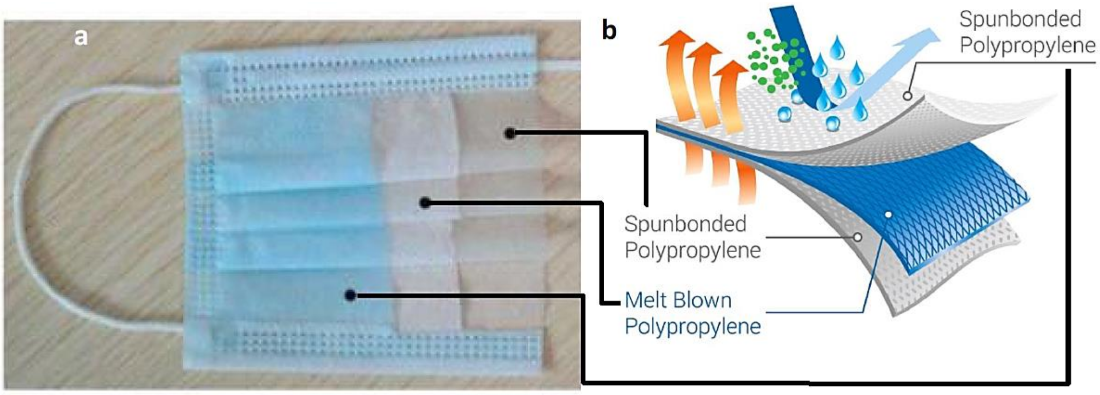

Fig. 4 Typical structure of a medical mask. Reproduced with the permission from [17], Copyright Engineered Science Publisher LLC 2020.

sterilization by ethylene oxide during the production process.

In addition to the aforementioned topics, there are still many more science and technology advancements on the way. We do hope this special issue could broaden the vision of readers and guide the new directions for these continuous developments in many years to come.

Conflict of interest

There are no conflicts to declare.

Supporting information

Not applicable.

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