VIDEO ARTICLE

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Digital-intellectual Design for Desired Materials

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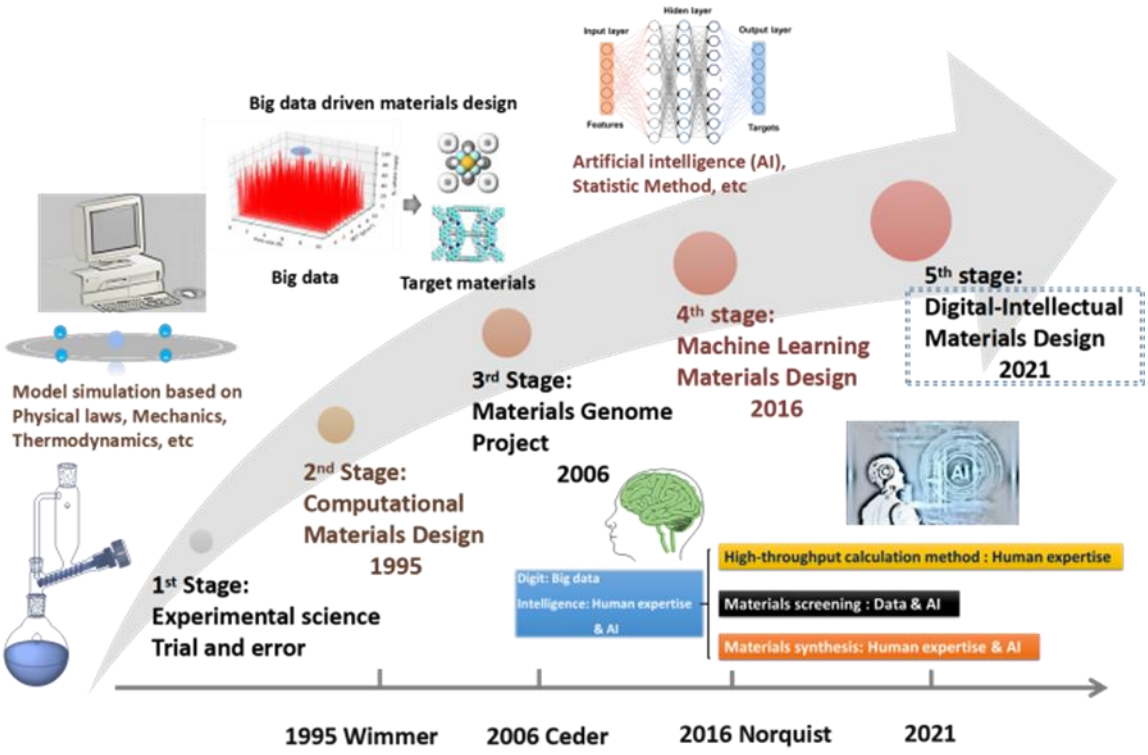
Graphical Abstract



Digital-Intellectual Design for Desired Materials.

Abstract

Traditional design strategy for new materials with targeted properties is trial-and-error method, which is time- and cost-consuming. In recent decades, computational materials design has been gaining rapid development including materials genome and machine learning. Recently, we proposed a digital-intellectual materials design method, in which digitization is embodied in big data and intelligence here means not only the wisdom of artificial intelligence (AI) but also human expertise. It requires the seamless integration of data, AI and especially human expertise [**1**]. This new way of materials design can be divided into three processes: development of a property prediction method, high-throughput material screening and retro synthesis of designed material. Here, I would introduce several cases of digital-intellectual design in the fields of porous materials, organic semiconductors and electrocatalyst, which have been achieved in our group recently. We developed a van der Waals force field for describing the adsorption of gas in porous materials [**2**] and used it to design and synthesize series of materials which can capture carbon dioxide and convert it to valuable chemicals at room temperature and atmospheric pressure [**3**]. Moreover, we developed a hole/electron mobility theory for describing incoherent charge transport in organic semiconductors [**4**] and used it to design series of organic

materials. Eventually, we developed a two-dimensional descriptor for oxygen evolution reaction and used it to screen and design covalent organic frameworks electrocatalysts [**5**]. With the rapid development of computational materials, we believe that the computation materials design especially digital-intellectual materials design may accelerate the materials discovery process.

Keywords: Computation simulation; materials design; carbon dioxide capture and conversion; new energy.

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Biography

Weiqiao Deng, Professor in Shandong University. I obtained my Ph.D degree in California Institute of Technology in 2004. From 2004 to 2019, I successively engaged in scientific research as Associate Researcher, Assistant Professor and Professor at California Institute of technology, Nanyang University of technology in Singapore and Dalian Institute of Chemical Physics, Chinese Academy of Sciences, respectively. In 2019, I joined the Institute of Frontier and Interdisciplinary Science in Shandong University as a Distinguished Professor. In 2015, I achieved The National Science Fund for Distinguished Young Scholars. In 2017, I was funded by the National Key Research & Development Program as the chief of the project. My research interest mainly focuses on the computational materials. By combining theory with experiment, my co-workers and I developed series of theoretical methods for property prediction, designed and synthesized series of desired materials for carbon capture, organic semiconductors and water splitting. I have published more than 200 SCI papers on *Nat. Commun.*, *J. Am. Chem. Soc.*, *Angew. Chemie. Int. Ed.*, e.g., which have been cited for more than 10,000 times with the H-index of 56.

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