

Machine Learning for Materials, a Journey from Artificial Intelligence to Intelligent Materials

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Invited Talk

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The design and synthesis of materials with useful, novel properties is one of the most active areas of contemporary science, generating a veritable explosion of scientific activity in areas such as biomaterials, cell and tissue engineering, organic photovoltaics and light-emitting materials, and nanomaterials for a myriad of medical and non-medical applications. This new era of materials design and discovery covers many disciplines from chemistry and biology to physics and engineering. Conventionally, it takes at least 20 years to move a material from initial discovery to the marketplace. To accelerate the pace of novel materials discovery, computational methods such as artificial intelligent machine learning techniques can be used to construct predictive materials property models and allow rapid scanning of large chemical datasets to systematically identify attractive candidates for specific applications. This presentation will showcase recent studies on data-driven design of functional materials for a broad spectrum of applications such as drug delivery, antifouling materials, and CO₂ capturing materials.

Keywords: