NANOBIOMAT-08: Nanotechnology & Biomaterials Sci. Congress, Birmingham & Portsmouth, UK-Jackson & Fargo, USA 2022.

Submit Now

Applications of Artificial Intelligence in nanoscience.

Shan He
Department of Organic and Inorganic Chemistry, Faculty of Science and Technology, University of the Basque Country UPV/EHU, P.O.Box 644, 48080 Bilbao, Spain.
IKERDATA S.L INVESTIGO Next-generation Researcher.

Abstract. Machine learning (ML) has gained extensive attention in recent years due to its powerful data analysis capabilities. It has been successfully applied to many fields such as chemical, pharmaceutical, biological etc. This powerful tool helped the researchers to achieve several major theoretical and applied breakthroughs. Some of the notable applications in the field of computational nanotechnology are ML potentials, property prediction, and material discovery. Therefore, In this review different type of application of machine learning in nanotechnology will be discussed.

There is currently no other hot topic like the ability of current technology to develop capabilities similar to those of human beings, even in medicine. This ability to simulate the processes of human intelligence with computer systems is known as artificial intelligence (AI).[1] One of the areas of AI is the technique of ML which has gained extensive attention in recent years due to its powerful data analysis capabilities. It has been successfully applied to many fields such as chemical, pharmaceutical, biological etc.[2] This powerful tool helped the researchers to achieve several major theoretical and applied breakthroughs. Some of the notable applications in the field of computational nanotechnology are ML potentials, property prediction, and material discovery.[3] As a consequence of evident achievements on a wide range of predictive tasks, ML techniques are attracting significant interest across a variety of stakeholders.[4] Therefore, In this review different type of application of machine learning in nanotechnology will be discussed.

Firstly, Sacha and Varona reviewed some usages of artificial intelligence (AI) in nanotechnology research in the context of interpreting scanning probe microscopy, the study of biological nanosystems, the classification of material properties at the nanoscale, theoretical approaches and simulations in nanoscience, and generally in the design of nanodevices. Current trends and future perspectives in the development of nanocomputing hardware that can boost artificial-intelligence-based applications are also discussed. Convergence between artificial intelligence and nanotechnology can shape the path for many technological developments in the field of information sciences that will rely on new computer architectures and data representations, hybrid technologies that use biological entities and nanotechnological devices, bioengineering, neuroscience and a large variety of related disciplines.[5]

Secondly, Liu *et al*. reviewed state-of-the-art research progress in these three fields. ML potentials bridge the efficiency versus accuracy gap between density functional calculations and classical molecular dynamics. For property predictions, ML provides a robust method that eliminates the need for repetitive calculations for different simulation setups. Material design and drug discovery assisted by ML greatly reduce the capital and time investment by orders of magnitude. In this perspective, several common ML potentials and ML models are first introduced. Using these state-of-the-art models, developments in property predictions and material discovery are overviewed. Finally, this paper was concluded with an outlook on future directions of data-driven research activities in computational nanotechnology.[3]

---

[1] Dorado-Díaz, P. I.; Sampedro-Gómez, J.; Vicente-Palacios, V.; Sánchez, P. L. Applications of artificial intelligence in cardiology. The future is already here. *Revista Española de Cardiología (English Edition)*, **2019**, *72*(12), 1065-1075.

[2] Simón-Vidal, L.; García-Calvo, O.; Oteo, U.; Arrasate, S.; Lete, E.; Sotomayor, N.; Gonzalez-Diaz, H. Perturbation-theory and machine learning (PTML) model for high-throughput screening of Parham reactions: experimental and theoretical studies. *Journal of Chemical Information and Modeling*, **2018**, *58*(7), 1384-1396.

[3] Liu, W.; Wu, Y.; Hong, Y.; Zhang, Z.; Yue, Y.; Zhang, J. Applications of machine learning in computational nanotechnology. *Nanotechnology*, **2022**, *33*(16), 162501.

[4] Mirzaei, M.; Furxhi, I.; Murphy, F.; Mullins, M. A Machine Learning Tool to Predict the Antibacterial Capacity of Nanoparticles. *Nanomaterials* **2021**, *11*, 1774.

[5] Sacha, G. M.; Varona, P. Artificial intelligence in nanotechnology. *Nanotechnology*, **2013**, *24*(45), 452002.

Lastly, Haick and Tang overviewed on the integration of nanotechnology-based medical sensors and AI for advanced clinical decision support systems to help decision-markers and healthcare systems improve how they approach information, insights, and the surrounding contexts, as well as to promote the uptake of personalized medicine on an individualized basis. Relying on these milestones, wearables sensing devices could enable interactive and involving clinical decisions that could be used for evidence-based analysis and recommendations as well as for personalized monitoring of diseases progress and treatment. In this context, these authors presented and discussed the ongoing challenges and future opportunities associated with AI-enabled medical sensors in clinical decisions.[6]

To conclude, as far as I am concerned, in the future the applications of machine learning and artificial intelligence on nanotechnology will be huge with promoting results as we saw previously. In fact, it is really useful tool not only in the field of nanoscience, but also in other research areas.

[6] Haick, H.; Tang, N. Artificial intelligence in medical sensors for clinical decisions. *ACS nano*, **2021**, *15*(3), 3557-3567.