Recapping 2020's Top Nanotechnologies for Life: Artificial Intelligence Can Now Reliably Predict Nanoparticle Structure and Dynamics

2021-02-07

Researchers at the University of Jyväskylä have recently shown that new distance-based machine learning methods can precisely predict the structures and atomic dynamics of nanoparticles in a faster manner compared to traditional simulation methods, and also facilitates Monte Carlo simulations of the atom dynamics of the particles at elevated temperatures.

Professor Tommi Kärkkäinen's group at the Nanoscience Center at the University of Jyväskylä has recently applied new distance-based machine learning methods applied to ligand-stabilized metal nanoparticles and published a method that is able to successfully predict binding sites of the stabilizing ligand molecules on the nanoparticle surface.

It describes each momentary atomic configuration of a nanoparticle by calculating a so-called descriptor and compares distances between descriptors in a multi-dimensional numerical space. By using correlations to a training set created by the reference DFT simulations, the potential energy can be predicted.

This approach, used now for the first time in nanoparticle research, is simpler and more transparent than traditionally used neural networks. The tool facilitates Monte Carlo simulations of the atom dynamics of the particles at elevated temperatures. The study was published in a Special Issue devoted to machine learning in The Journal of Physical Chemistry in 2020.

The potential energy of a system is a fundamental quantity in computational nanoscience since it allows for the quantitative evaluations of the system's stability, rates of chemical reactions, and strengths of interatomic bonds. Ligand-stabilized metal nanoparticles have many types of interatomic bonds of varying chemical strength, and traditionally the energy evaluations have been done by using the so-called density functional theory (DFT) that often results in numerically heavy computations requiring the use of supercomputers.

The researchers used the potential energies, predicted by the machine learning method, to simulate the atomic dynamics of thiol-stabilized gold nanoparticles. The results were in good agreement with the simulations performed by using the density functional theory. This new method allowed simulations to be run on a laptop or desktop in a time scale of a few hours while the reference DFT simulations took days in a supercomputer and used simultaneously hundreds or even thousands of computer cores. The speed-up will allow long-time simulations of the particles' structural changes and particle-particle reactions at elevated temperatures.

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