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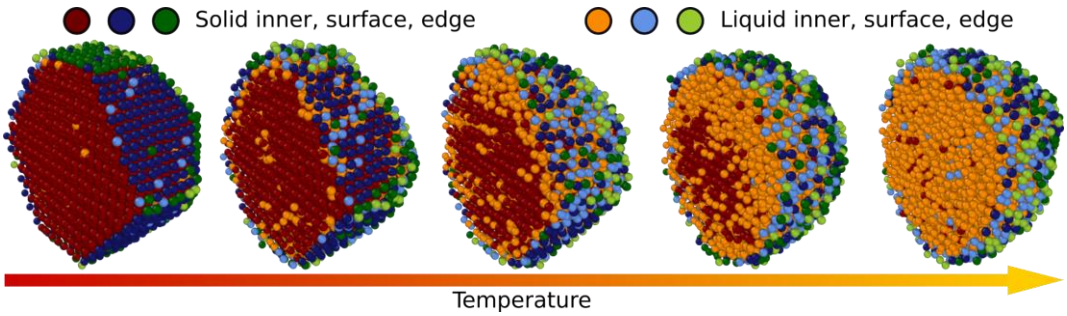
PRESS RELEASE

Gold nanoparticle melting: a data driven simulation

In a new study, machine learning has been used to simulate and analyze the state of gold nanoparticles - an important technological material - at high temperatures. The findings have been published in Nature Communications.



Trieste, 9 November 2021

Gold nanoparticles' have unique properties, which make them relevant in catalysis, biomedicine, and optics. These properties dramatically change depending on whether the nanoparticles, and their surface, are in a liquid or solid state.
A mechanistic picture of the melting mechanism of small (few nanometers wide) gold particles, as well as a tool to quantitatively predict their melting temperature, is therefore key for their application in cutting-edge technologies. Unfortunately, classical thermodynamics fails in these systems because of the importance of complex surface effects at the nanoscale.

An international study led by SISSA, in collaboration with the École Polytechnique Fédérale de Lausanne, King's College London, Swansea University and the Aristotle University of Thessaloniki, used machine learning to address the challenge of accurately predicting and characterizing the temperature-dependent phase of small gold nanoparticles. The use of machine learning to predict the forces acting on atoms in the nanoparticles allowed the researchers to quickly conduct long simulations with quantum-mechanical precision. The article has been published in Nature Communications

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“Simulations that would have taken thousands of years to compute if done with traditional Density Functional Theory methods, can be performed in a few days by using machine learning force fields” says Claudio Zeni, first author of the research.

Data-driven methods have also been applied to analyse these long simulations. As the authors explain: “Unsupervised learning, in conjunction with state-of-the art methods to encode what the surroundings of an atom look like, allowed us to automatically label each atom as in a liquid or solid state, and as a surface, edge, or core atom. This sped up the analysis and provided an unbiased framework to discriminate when surface rearrangement, a phenomenon that plays an important role in the functionality of small nanoparticles, takes place.”

The techniques developed and employed in the article can be applied to a vast array of technologically important systems, and the authors foresee many alleys to improve and standardize the approach.

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Full paper:
https://www.nature.com/articles/s41467-021-26199-7

IMAGE
Crediti: **Claudio Zeni**

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