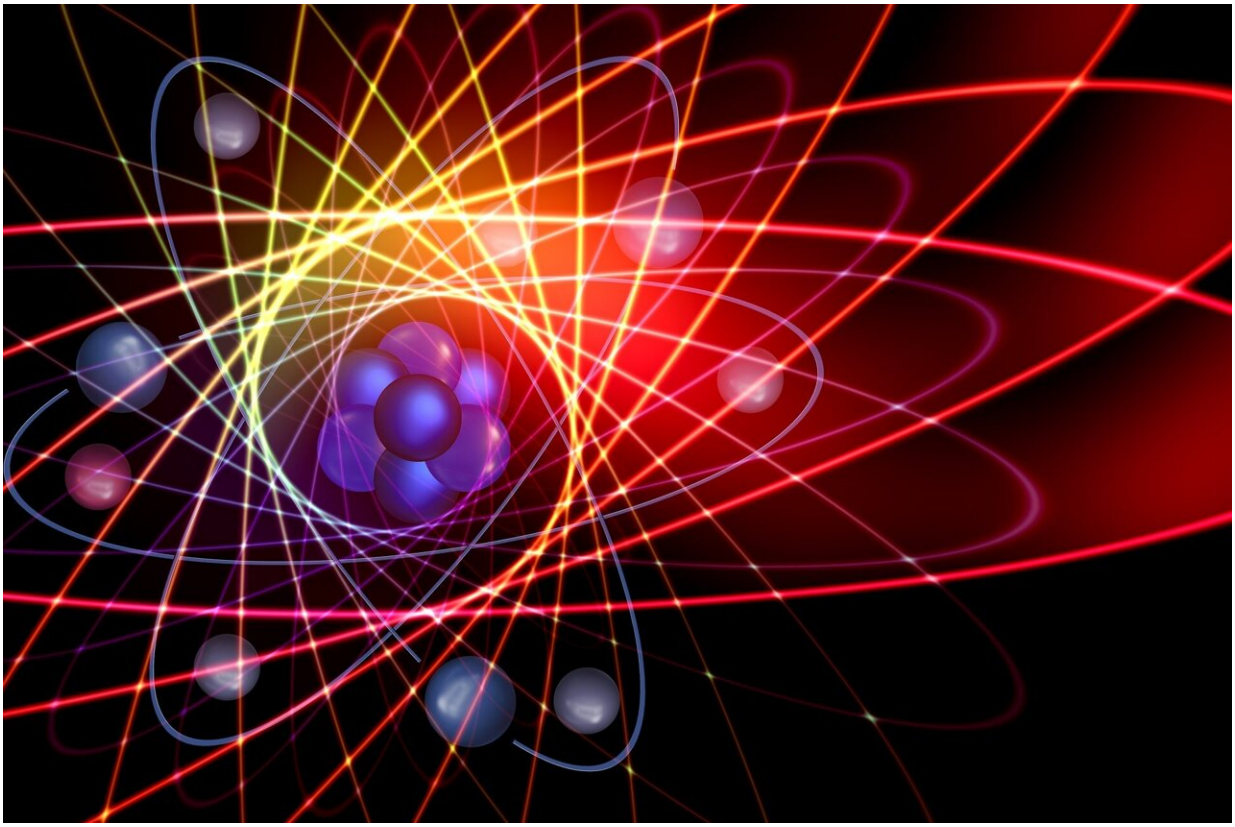
Online library helps advance nanomaterial development

July 9 2021



Credit: Pixabay/CC0 Public Domain

NMs have made their way into our lives and are helping to improve—even revolutionize—many industries. In the cosmetics industry, mineral nanoparticles help create sunscreens that provide

improved protection from the sun's harmful rays. In sports, carbon nanotubes make for lighter and better baseball bats. Benefits for healthcare include more effective drug delivery to affected areas of the body. These examples are just the tip of the iceberg. NMs are also finding uses in the electronics, energy, construction, automotive and defense sectors, to name a few.

But what about their possible adverse effects? Although NMs are benefiting us in many ways, there are also concerns about the little information available on how exposure to these materials may affect people and the environment. To address this problem, the EU-funded NanoSolveIT project is introducing a novel Integrated Approach to Testing and Assessment (IATA) for NMs. The IATA will be used to identify the critical characteristics of NMs responsible for their adverse effects on human health and the environment, or for their functionalities in high-tech applications. It will furthermore be implemented as a decision support system presented via stand-alone open-source software and a cloud platform.

Dr. Antreas Afantitis, managing director of Cypriot in silico drug design company and NanoSolveIT project coordinator NovaMechanics Ltd, talks about the project's achievements so far: "In the last two years, the project has already presented some very impressive results with more than 30 publications, making the project one of the most active in the NMs space," he notes in a news release posted on the EIN Presswire website. One of these achievements is a freely available online library containing the complete physical and chemical characteristics of 69 NMs, as well as calculated molecular descriptors that increase the value of the available information.

Reliable data for NM characterization

With over 70 descriptors per NM, the rich data set was used to develop

an in silico workflow to predict the zeta potential, or effective surface charge, of NMs. This prediction was based on descriptors that can be used as part of a safe-by-design approach that includes safety at the earliest possible stage of NM development to prevent health and environmental risks.

"One of the limitations to the widespread application of in silico approaches is the lack of large quantities of high-quality data, or of data with adequate metadata that will allow dataset interoperability and their combination to create larger datasets," observes Prof. Iseult Lynch of NanoSolveIT project partner University of Birmingham in the same news release. The project is helping to meet this need by making the library of calculated and experimental descriptors, as well as details on how descriptors were calculated (presented in MODA template format), freely available to researchers and interested stakeholders.

The read-across zeta potential predictive model is available as a web service via the NanoSolveIT Cloud Platform as well as the EU-funded project NanoCommons. This is a key step in the NanoSolveIT (Innovative Nanoinformatics models and tools: towards a Solid, verified and Integrated Approach to Predictive (eco)Toxicology (NanoSolveIT)) project's ambition to create accessible, user-friendly and reliable nanoinformatics models that will remove barriers from nanosafety-related regulatory and industrial processes.

More information: NanoSolveIT project website: nanosolveit.eu/

Provided by CORDIS