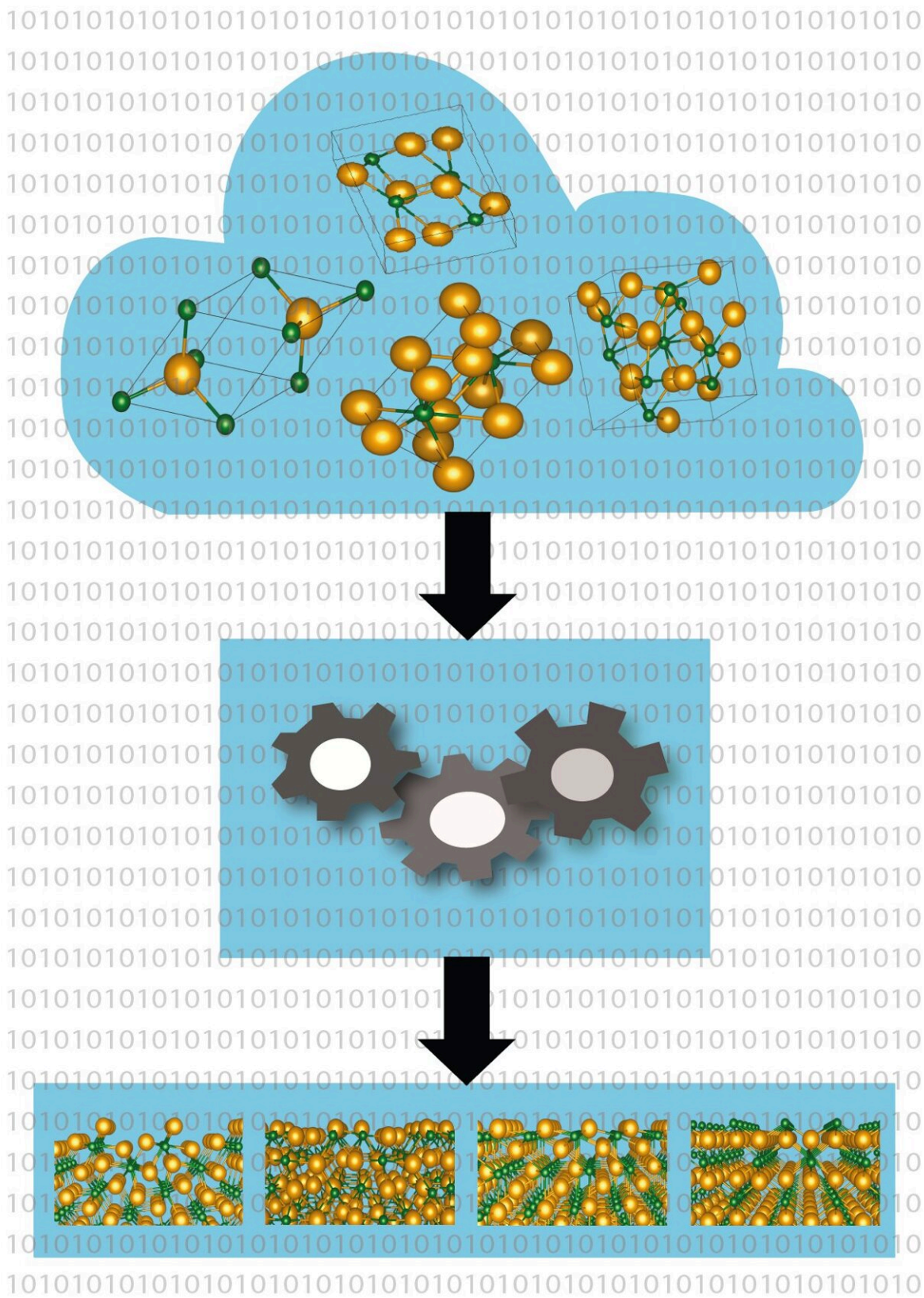


New method provides automated calculation of surface properties in crystals

March 28 2024



Based on a small amount of basic information about a crystal's structure, the Oldenburg researchers' program calculates the properties of complex new materials. Credit: University of Oldenburg / EST group

Computer-based methods are becoming an increasingly powerful tool in the search for new materials for key technologies such as photovoltaics, batteries, and data transmission. Prof. Dr. Caterina Cocchi and Holger-Dietrich Saßnick from the University of Oldenburg in Germany have now developed a high-throughput automatized method to calculate the surface properties of crystalline materials starting directly at the level of established laws of physics (first principles).

In an article [published](#) in the journal *npj Computational Materials*, they report that this can speed up the search for relevant materials for applications in key areas such as the energy sector. They also plan to combine the method with [artificial intelligence](#) and machine learning techniques to accelerate the process further.

So far, similar methods have focused on bulk materials rather than surfaces, the two physicists explain. "All the relevant processes for energy conversion, production, and storage occur on surfaces," says Cocchi, who heads the Theoretical Solid State Physics research group at the University of Oldenburg.

However, calculating the material properties of surfaces is far more challenging than for complete crystals because the surface facets often have a complex structure due to factors such as defects in the [crystal structure](#) or the uneven growth of a crystal, she explains.

This complexity poses problems for researchers in the field of materials

science: "It is often not possible to clearly determine the properties of samples in experiments," says Cocchi. This motivated Cocchi and her colleague Saßnick to develop an automated procedure for high-quality screening of the characteristics of new compounds.

Reliable results

The result of their work was incorporated into the aim2dat computer program, which only requires the chemical composition of a compound as input. The information about the crystal's structure is extracted from existing databases. The software then calculates the conditions under which the surface of the material is chemically stable.

In the second step, it determines key properties, in particular, the energy required to excite electrons into conduction states or detach themselves from a surface. This parameter plays an important role in materials that convert solar energy into electricity, for example. "We don't make any assumptions in our calculations; we use only the fundamental equations of quantum mechanics, which is why our results are very reliable," Cocchi explains.

The two scientists demonstrated the applicability of the method using the semiconductor cesium telluride. The crystals of this material, which are used as an electron source in [particle accelerators](#), can occur in four different forms. "The composition and quality of the material samples are difficult to control in experiments," notes Saßnick. Nevertheless, the Oldenburg researchers were able to perform a detailed analysis of the physical properties of the different configurations of the cesium telluride crystals.

Cocchi and Saßnick have embedded the software in a publicly accessible program library so that other researchers can also use and improve the procedure. "Our method has great potential as a tool for discovering new

materials—and in particular physically and structurally complex solids—for all kinds of applications in the [energy sector](#)," says Cocchi.

More information: Holger-Dietrich Saßnick et al, Automated analysis of surface facets: the example of cesium telluride, *npj Computational Materials* (2024). [DOI: 10.1038/s41524-024-01224-7](https://doi.org/10.1038/s41524-024-01224-7)

Provided by University of Oldenburg

Citation: New method provides automated calculation of surface properties in crystals (2024, March 28) retrieved 9 May 2024 from <https://phys.org/news/2024-03-method-automated-surface-properties-crystals.html>

<p>This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.</p>
--