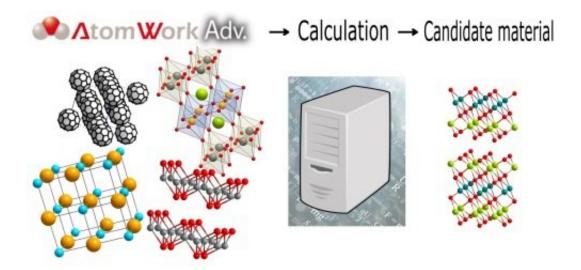


## Using big databases to find superconductors of the future

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A data-driven approach helps identify superconducting materials. Credit: National Institute for Materials Science

Japanese researchers have found an approach to more quickly and successfully identify superconducting materials.

"The data-driven approach shows promising power to accelerate the discovery of new thermoelectric and <u>superconducting materials</u>," the researchers say in their study published in the journal *Science and Technology of Advanced Materials*.

Superconductors are materials that conduct electricity with virtually no



resistance. Superconducting materials have improved the field of magnetic resonance imaging (MRI) and have led to the development of particle colliders that can be used for research related to splitting atoms. Currently available superconducting materials can only perform at extremely low temperatures. If researchers can find superconducting materials that work at ambient temperature, electricity could be conducted over large distances without energy loss.

Current approaches to searching for these materials are somewhat random, and results strongly depend on researcher's intuition, experience and luck. Materials scientist Yoshihiko Takano of Japan's National Institute for Materials Science and colleagues have shown that sifting through an inorganic materials database using specific search parameters can provide a more systematic way to finding superconducting materials.

They searched through AtomWork, a large database for inorganic materials. In a previous study using this same approach, the team identified  $\text{SnBi}_2\text{Se}_4$  (a compound of tin, bismuth, and selenium) as a potential superconductor. Experiments showed that this was indeed the case.

But  $\text{SnBi}_2\text{Se}_4$  requires very low temperatures and high pressures to become superconductive. The team searched once more through the database, selecting <u>materials</u> that have a similar crystal structure to  $\text{SnBi}_2\text{Se}_4$  but a narrower 'band gap', a property related to atomic structure that allows electrons to jump up from one energy level to another and thus partake in electrical conductivity.

Their best choice was  $PbBi_2Te_4$  (formed of lead, bismuth, and tellurium). They synthesised  $PbBi_2Te_4$  crystals, examined their structure, chemical composition and other properties, and found that those properties met the predictions. They exposed the crystals to high pressures and varying temperatures and found that the electrical



resistance of  $PbBi_2Te_4$  decreased with increasing pressure, reaching a superconductive state at 10 gigapascals, about half the pressure needed for  $SnBi_2Se_4$  to become superconductive.

"This work presents a case study for the important first-step for the nextgeneration data-driven <u>materials science</u>," the team concludes.

**More information:** Ryo Matsumoto et al. Data-driven exploration of new pressure-induced superconductivity in PbBi<sub>2</sub>Te<sub>4</sub>, *Science and Technology of Advanced Materials* (2018). DOI: 10.1080/14686996.2018.1548885

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