

Scientists discover a new complex europium hydride

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Credit: Journal of Physical Chemistry Letters

A team of researchers from Russia, the United States and China led by Skoltech Professor Artem R. Oganov have discovered an unexpected very complex europium hydride, Eu_8H_{46} . The paper detailing the discovery has been published in the *Journal of Physical Chemistry letters*.



Superhydrides of rare-earth metals are interesting compounds that form under pressure: Some exhibit high-temperature superconductivity that scientists have been chasing for over 100 years, and some possess magnetic properties. Although devoid of superconductivity, europium hydrides are very interesting in view of chemical anomalies that make <u>europium</u> different from other rare earth atoms.

Armed with the efficient and reliable USPEX crystal structure prediction tool developed by Oganov and his students, the team predicted the structure of the remarkably complex compound Eu_8H_{46} , which helped explain the experimental data.

"I am pleasantly surprised that USPEX has easily predicted a highly complex structure of 54 atoms, which is quite a lot. Curiously enough, our colleagues obtained this hydride in experiment earlier but got the structure and composition wrong, assuming it was EuH₅. Now we know that the compound is much trickier," Oganov comments.

"Such unusual compounds can be predicted in theory and proved by experiment, but there is no simple rule for identifying probable chemical compositions of stable <u>compounds</u> without performing arduous calculations," says Dmitrii Semenok, the first author of the paper and a Ph.D. student at Skoltech.

More information: Dmitrii V. Semenok et al. Novel Strongly Correlated Europium Superhydrides, *The Journal of Physical Chemistry Letters* (2020). DOI: 10.1021/acs.jpclett.0c03331

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