

New crystal structure for hydrogen compounds for high-temperature superconductivity

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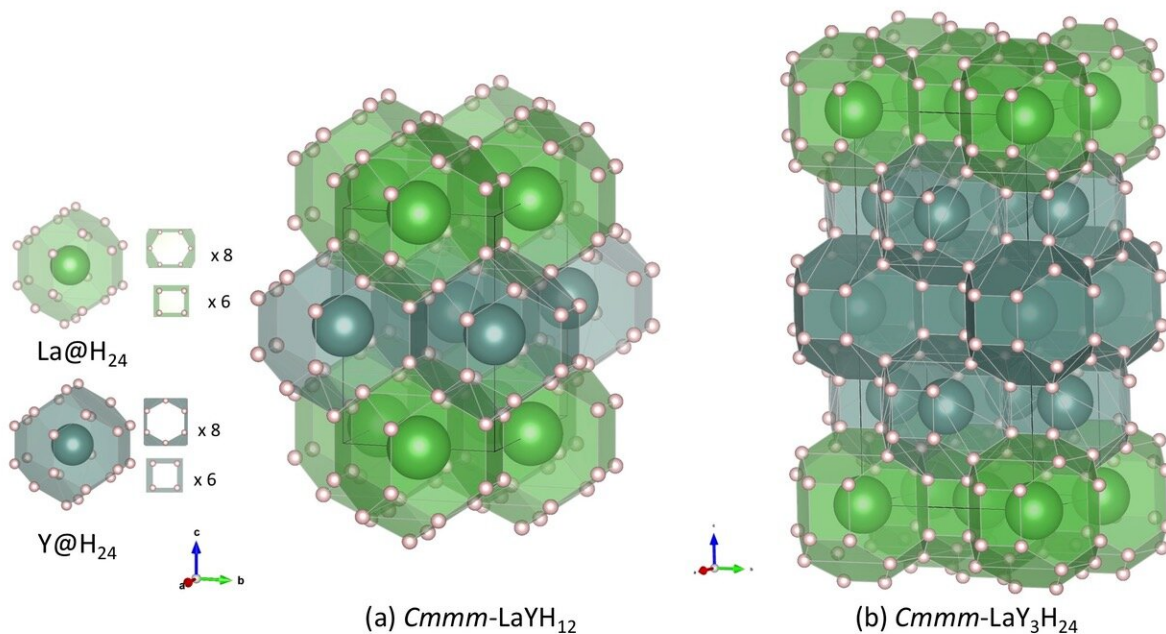


Figure 1. Clathrate structures of LaYH₁₂ and LaY₃H₂₄. Using computer simulations, a global team of researchers have predicted new crystal structures for realizing a high-temperature superconductor with ternary hydrides, a step toward realizing a low-cost and lossless power transmission technology. Credit: Ryo Maezono from JAIST.

Superconductivity is the disappearance of electrical resistance in certain

materials below a certain temperature, known as "transition temperature." The phenomenon has tremendous implications for revolutionizing technology as we know it, enabling low-loss power transmission and maintenance of electromagnetic force without electrical supply. However, superconductivity usually requires extremely low temperatures ~ 30 K (the temperature of liquid nitrogen, in comparison, is 77 K) and, therefore, expensive cooling technology. To have a shot at realizing a low-cost superconducting technology, superconductivity must be achieved at much higher transition temperatures.

Materials scientists have had a breakthrough on this front with crystalline materials containing hydrogen, known as "metal hydrides." These are compounds formed by a metal atom bonded with hydrogen that have been predicted and realized as suitable candidates for achieving even room-temperature superconductivity. However, they require extremely high pressures to do so, limiting their practical applications.

In a new study published in *Chemistry of Materials*, a group of researchers led by Professor Ryo Maezono from Japan Advanced Institute of Science and Technology (JAIST) performed [computer simulations](#) to expand the search for high-temperature superconductors, looking for [potential candidates](#) among ternary hydrides (hydrogen combined with two other elements).

"In ternary hydrides, the number of elements is increased from two to three. While this enormously increases the number of possible combinations and can make the problem of predicting suitable materials more difficult, it also increases our chances of coming across a potential high-temperature superconductor," explains Prof. Maezono.

Using the supercomputer at the university, the researchers examined

possible crystal structures for (LaH₆) (YH₆)_y compounds (y= 1–4), looking for configurations that would yield stable structures, allowing their synthesis in the laboratory at high pressures. Starting from a random structure, the simulations went through various possible combinations of elements, testing their stability at extremely high pressures ~ 300 GPa.

The simulations revealed clathrate (Cmmm-) structures of LaYH₁₂ and LaY₃H₂₄, consisting of LaH₂₄ and YH₂₄ cages stacked on top of each other (Figure 1), as viable candidates for high-temperature and [high-pressure](#) superconductors. "The longer stacking for Cmmm-LaY₃H₂₄ lead to a slightly increased [transition temperature](#)," explains Prof. Maezono. Among the possible structures, the highest transition temperature (145.31 K–137.11 K) was observed for LaY₃H₂₄. The researchers attributed the origin of higher transition [temperature](#) to a high "density of states" and high "phonon frequency," two parameters that are used to assess superconductivity in materials.

These findings have excited the researchers, who optimistically speculate the discovery of more such [high-temperature superconductors](#). "It is quite possible to predict using simulations other new combinations of elements that would improve the desired properties further," says Prof. Maezono.

More information: Peng Song et al, High-Tc Superconducting Hydrides Formed by LaH₂₄ and YH₂₄ Cage Structures as Basic Blocks, *Chemistry of Materials* (2021). [DOI: 10.1021/acs.chemmater.1c02371](https://doi.org/10.1021/acs.chemmater.1c02371)

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