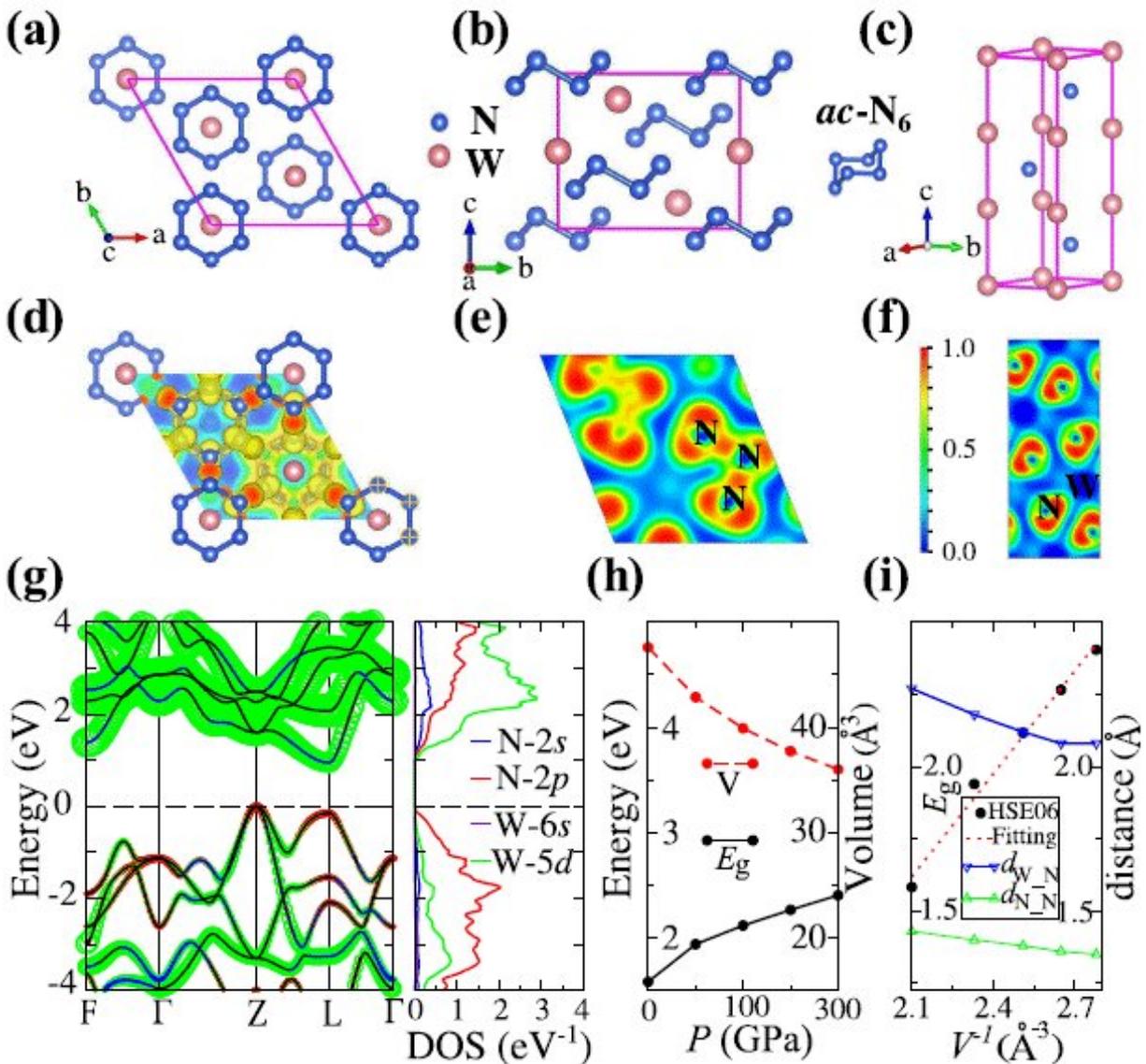


Machine learning predicted a superhard and high-energy-density tungsten nitride

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Crystal structure and theoretical electronic structures of new W-N phases.

Credit: ©Science China Press

Although machine learning has been successful in many aspects, its application in crystal structure predictions and materials design is still under development. Recently, Prof. Jian Sun's group at the Department of Physics, Nanjing University, implemented a machine-learning algorithm into the crystal structure search method. They used a machine learning algorithm to describe the potential energy surface and used it to filter the crystal structures, enhancing the search efficiency of crystal structure prediction.

Hybrid compounds of transition metals and [light elements](#), especially transition metal nitrides, have been widely studied for their high incompressibility and bulk modulus. However, superhard tungsten nitrides (Vickers hardness over 40 GPa) have not yet been found. The energy bands contributed by d valence electrons of tungsten atoms can easily cross the fermi energy level, and the metallicity leads to great reduction of their hardness. Therefore, designing non-metallic tungsten nitride crystal structures seems be a promising way to reach outstanding mechanical properties such as super-hardness.

Based on previous research, a collaboration led by Prof. Jian Sun and Prof. Hui-Tian Wang at Department of Physics, Nanjing University, summarized three traits for designing superhard hybrid compounds of transition metal and light elements: high-pressure stable and ambient-pressure metastable crystal structure, non-metallic electronic structures, and a large ratio of light elements. These characteristics inspired them to design nitrogen-rich tungsten nitrides containing special nitrogen-based basic configurations, such as rings, chains, networks and frameworks, etc. Based on these design rules and the newly developed machine-learning crystal structure search method, they have successfully

predicted a non-metallic nitrogen-rich tungsten nitride h-WN6. It has a sandwich-like structure formed by nitrogen six-membered ring and tungsten atoms.

The electron localization function and Bader charge analysis indicate that h-WN6 is an ionic crystal containing strong N-N covalent bonds. It can be stable at high pressures and metastable at ambient pressure. Moreover, it has a small, indirect energy-gap and abnormal gap broadening behavior under compression. (see the crystal [structure](#), electronic structures and the high pressure behaviors in the attached figure). More interestingly, h-WN6 is estimated to be the hardest among transition metal nitrides known so far, with a Vickers hardness around 57 GPa and also has a pretty high melting temperature of around 1,900 K. Moreover, their calculations also show that this nitrogen-rich compound can be considered as a potential high-energy-density material because of the good gravimetric (3.1 kJ/g) and volumetric (28.0 kJ/cm³) energy densities.

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A collaborated research team from China implemented a machine-learning algorithm into the crystal structure search method and found a superhard tungsten nitride by using their new method. Their calculations show that this compound is the hardest transition metal nitride known so far, and it also has other extraordinary properties, such as high melting temperature and high-energy-density. Credit: ©Science China Press

The researchers developed a machine learning accelerated [crystal structure](#) search method, summarized the design rules of superhard transition metal light elements compounds, and predicted a superhard and high-energy-density [tungsten](#) nitride with good thermal stability. The study will stimulate the theoretical design and experimental synthesis of this kind of [transition metal](#) material with potential application value. This will also enrich the family of superhard materials and may be used a reference for understanding the origin of hardness.

More information: Kang Xia et al, A novel superhard tungsten nitride predicted by machine-learning accelerated crystal structure search, *Science Bulletin* (2018). [DOI: 10.1016/j.scib.2018.05.027](https://doi.org/10.1016/j.scib.2018.05.027)

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