# AI-empowered discovery of novel materials for smart electronic devices

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## 1. AI in materials science

In recent years, the demand for novel materials and algorithms for designing materials with target properties has been steadily increasing. The ever-growing industrial requirements for material quality and performance, along with the high cost of experimental discovery, serve as the primary motivation for advancing computational materials science and materials informatics. Traditionally, new materials have been explored through experimental methods, where novel compositions or synthesis conditions were proposed based on the accumulated expertise of individual researchers or previous experimental results. However, this approach is time-consuming, requires specialized experimental facilities, and depends on the experience of experimentalists. In contrast, over the past two decades, computational materials design methods have seen significant progress, enabling the accurate prediction of material structures and properties before their physical synthesis or experimental testing.

Moreover, the integration of AI algorithms has significantly accelerated the discovery of new materials. The development of large-scale materials databases [1], machine learning methods for predicting properties based on composition and structure [2], and generative algorithms for designing novel materials have further enhanced the efficiency and accuracy of materials research [3]. These advancements pave the way for a more systematic and data-driven approach to materials discovery and innovation.

## 2. How AI changes the way of materials discovery

In the presented talk we will demonstrate how machine learning methods are already being employed for the discovery of new materials capable of altering the properties and expanding the application domains of electronic and photonic devices.

The exploration of van der Waals (vdW) materials, renowned for their unique optical properties, is pivotal for advanced photonics. These materials exhibit exceptional optical anisotropy, both in-plane and out-of-plane, making them an ideal platform for novel photonic applications. However, the manual search for vdW materials with giant optical anisotropy is a labor-intensive process unsuitable for the fast screening of materials with unique properties. Here, we collected a database of vdW materials and their optical properties [4-6] and trained graph neural network to predict their birefringence with close to ab initio accuracy. Experimental verification with 2H-MoTe2 and CdPS3 confirms the theoretical predictions, underscoring the potential of ML in discovering and optimizing vdW materials with unprecedented optical performance [7].

Two-dimensional materials have attracted considerable attention due to their remarkable electronic, mechanical and optical properties, making them prime candidates for next-generation electronic and optoelectronic applications. Here we developed a novel method for predicting the atomic structure of 2D materials on arbitrary substrates by combining an evolutionary algorithm, a lattice-matching technique, an automated machine learning interatomic potentials training protocol, and the ab initio thermodynamics approach for predicting the possible conditions of experimental synthesis of the predicted 2D structures. Using the Mo-S system on a c-cut sapphire substrate as a case study, we reveal several new stable and metastable structures, including previously known 1H-MoS2 and newly found Mo3S2, Mo2S, Mo5S3, and Mo4S (Fig. 1). These results provide insights into computational substrate engineering, allowing one to study the substrate effect on the thermodynamic and dynamical stability of 2D materials and to modulate their electronic and phonon properties for their future applications, as well as to provide guide maps for their experimental synthesis [8].

Finally, the latest results on the development of diffusion models for materials generation will be presented. Generative modeling is changing the traditional material discovery process by applying machine learning to predict and create new materials. These models use step-by-step processes to transform random noise into meaningful structures, making them a good match for generating complex 3D spatial structures like crystals.

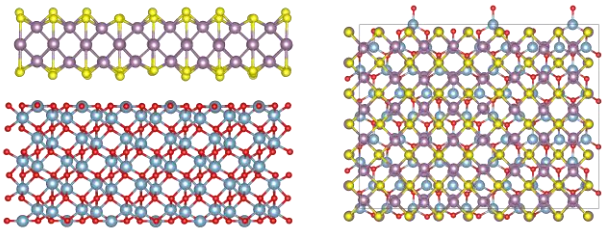

Fig. 1: Crystal structure of newly found $Mo_2S$ 2D-material.

## References

[1] Zagorac, D., Müller, H., Ruehl, S., Zagorac, J., & Rehme, S. (2019). Recent developments in the Inorganic Crystal Structure Database: theoretical crystal structure data and related features. Journal of applied crystallography, 52(5), 918-925.

[2] Choudhary, K., & DeCost, B. (2021). Atomistic line graph neural network for improved materials property predictions. npj Computational Materials, 7(1), 185.

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[3] Zeni, C., Pinsler, R., Zügner, D., Fowler, A., Horton, M., Fu, X., ... & Xie, T. (2025). A generative model for inorganic materials design. Nature, 1-3.

[4] Ermolaev, G. A., Grudinin, D. V., Stebunov, Y. V., Voronin, K. V., Kravets, V. G., Duan, J., ... & Volkov, V. S. (2021). Giant optical anisotropy in transition metal dichalcogenides for next-generation photonics. Nature communications, 12(1), 854.

[5] Ermolaev, G. A., Voronin, K. V., Toksumakov, A. N., Grudinin, D. V., Fradkin, I. M., Mazitov, A., ... & Novoselov, K. S. (2024). Wandering principal optical axes in van der Waals triclinic materials. Nature communications, 15(1), 1552.

[6] Slavich, A. S., Ermolaev, G. A., Tatmyshevskiy, M. K., Toksumakov, A. N., Matveeva, O. G., Grudinin, D. V., ... & Novoselov, K. S. (2024). Exploring van der Waals materials with high anisotropy: geometrical and optical approaches. Light: Science & Applications, 13(1), 68.

[7] Bereznikova, L. A., Kruglov, I. A., Ermolaev, G. A., Trofimov, I., Xie, C., Mazitov, A., ... & Novoselov, K. S. (2025). Artificial intelligence guided search for van der Waals materials with high optical anisotropy. Materials Horizons.

[8] Mazitov, A., Kruglov, I., Yanilkin, A. V., Arsenin, A. V., Volkov, V. S., Kvashnin, D. G., ... & Novoselov, K. S. (2024). Substrate-aware computational design of two-dimensional materials. arXiv preprint arXiv:2408.08663.