

Welcome to AIS-Square!

AI & Science Square (AIS-Square) is a collaborative and open-source platform for sharing AI4S datasets, models, and workflows, jointly developed by the Beijing Institute of Science and Intelligence (AISI), Deep Modeling community, and DP Technology Co., Ltd. Centered on the principles of "openness, collaboration, and sharing," AIS-Square aims to bring together outstanding scientists and industrial developers worldwide to exchange experiences in deep learning and physical modeling. Through cooperative sharing, we hope to drive the development of the entire scientific computing field, establish a more open and collaborative ecosystem, activate collaborative models in scientific research, and promote the application of more industrial scenarios.

About the name AIS-Square

In the name of AIS-Square, "AI" represents both "ab initio" and "artificial intelligence." "Square" refers to both "plaza" and $(AI)^2$, embodying the concept of co-construction, co-creation, and co-growth. The "square" also represents a unified platform for gathering wisdom and sharing contributions.

Little Spark, Deep Flame

The future is coming, and AI4S is becoming more and more popular. AI is empowering basic scientific exploration, helping scientists simulate the quantum behavior of particles at the microscopic scale and gain insights into the nature of the material world from the first principles. AIS-Square has already obtained and shared more than 300 million core-hours of computing resources, simulation and modeling data covering various application fields, over 50 specialized models for specific scenarios, complete dp-library content, pre-trained models such as Uni-Mol, and the world's first deep potential atomic potential energy function pre-trained model DPA-1 that covers nearly 70 elements. It has also accumulated cloud-native scientific computing automation processes such as material structure, mechanics, thermodynamic property calculations, and engine spray combustion simulations. In the future, users can also achieve more innovative functions such as multi-task training, model distillation, and model compression based on this platform. Various downstream task systems, such as alloys, semiconductors, and solid-state electrolytes, can also achieve one-click automated testing of models, further facilitating scientific research, promoting the development and application of scientific computing in various systems, and accelerating the pace of original innovation.

We look forward to your support and contribution.

【AISI】 <https://www.aisi.ac.cn/>

【Deep Modeling】 <https://deepmodeling.com/>

【Github discussions】 <https://github.com/deepmodeling/AIS-Square/issues>

【Contact us】 aissquare@bjaisi.com

AIS-square, working with ecological partners, provides a continuous stream of innovative vitality for the AI for Science field.