

自分だけの材料を作ろう！ 計算科学入門

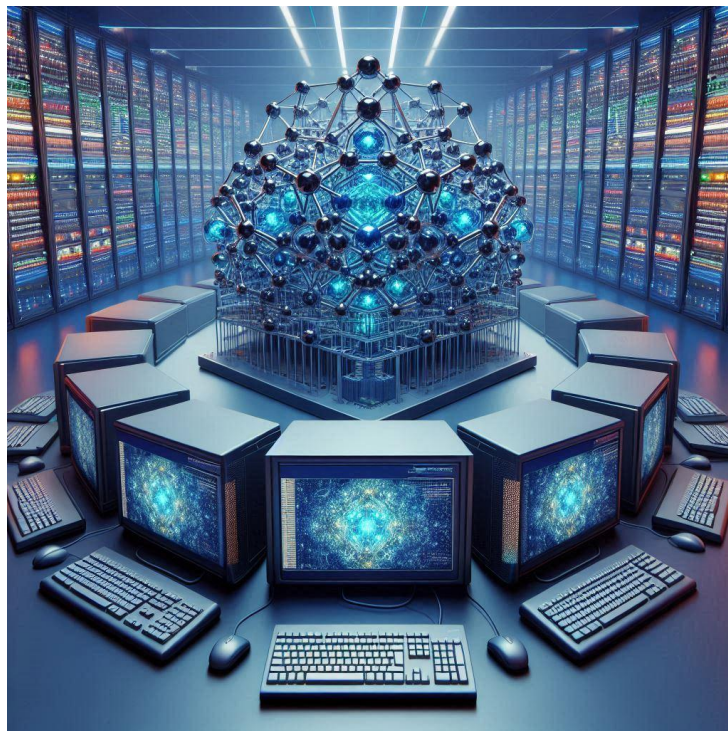
Create Your Own Material! An Introduction to First Principles Calculation

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With the advancement of science and technology, high-performance computers—so-called

supercomputers—play an increasingly important role in various fields. Japan's world-renowned supercomputer “京” began operation in 2011 and was ranked the fastest in the world at the time. It made major contributions in areas such as weather forecasting, earthquake simulation, and drug discovery. Its successor, “富岳,” started operation in 2020 and boasts approximately 100 times the computing power of 京. 富岳 has been widely used in fields including simulations to curb the spread of COVID-19, climate change prediction, and AI research. In this way, computer-based simulations have become increasingly relevant to our daily lives.



In this course, as an introduction to computational science, you will have the opportunity to design your own material and calculate its properties using a high-performance computer.

Through this training, students will experience the integration of materials science and computational science and gain an understanding of the significance and potential of computer simulations in modern research. The course particularly aims to help students develop the following skills—take your first step toward becoming a future researcher!

- Fundamentals of crystal structures and materials science
- Crystal design and computer simulation techniques
- Introductory quantum mechanics
- Data analysis and presentation skills