

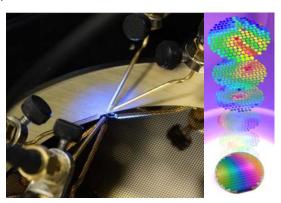
### Al Technology opens up next generation nanotech

### **Materials Informatics**

Automated processes using AI and robots will be a powerful and captivating tool also in the field of nanotechnology. On the other hand, it is still difficult that these systems understand this deep and wide field comprehensively only by themselves. NEC offers the explainable AI technology that enables human and AI to cooperatively figure out a way to proceed in the nanotechnology research field of enormous dimensions.

## ■Batch processes for combinatorial materials data set acquisition

The overarching issue in exploring new materials with data-driven approaches is how we acquire big data from a wide variety of materials. We utilize advantageous combinatorial technology that can exhaustively carry out experiments and simulations over possible combinations of candidate materials.

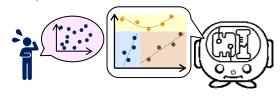


#### Automated big data processing using Al

What kind of physics is hidden behind the experimental data? A lot of experiments and simulations are required to clarify this, and a lot of data are produced. Our AI technology can handle various materials data such as worksheets, spectrum and image etc. and process feature extraction or clustering more rapidly and precisely than a bunch of scientists do.

#### Descriptor search using Heterogeneous Mixture Learning

The Heterogeneous Mixture Learning is one of the Explainable AI technologies that can give a result of analysis in a simple and readable form. In HML, classification and regression are simultaneously optimized for mixed and bulky data set such as combinatorial experiments, physical property simulations etc. The analysis also gives reference to certain parameters possibly to be identified as a descriptor for the test system.



# Rapid screening and optimization using Bayesian tree search

Once we define a target parameter or a descriptor to be optimized, AI technology helps the processes will proceed quickly and efficiently. Our Bayesian tree search algorithm can accomplish optimization of parameters defined in a super-multidimensional search space, where the optimization is hard to proceed with the conventional Gaussian process or upper bound

algorithm.

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