Empowering researchers to discover and develop new materials.

How **Skoltech** accelerates cutting-edge materials-science research with a new high-performance computing cluster based on Lenovo ThinkSystem SD530 servers and 2nd Gen Intel® Xeon® Scalable processors.

Lenovo Infrastructure Solutions for The Data-Centered

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Background

The Skolkovo Institute of Science and Technology (Skoltech) is a private graduate research university in Moscow, Russia. Established in 2011 in collaboration with the Massachusetts Institute of Technology (MIT), Skoltech educates global leaders in innovation, advances scientific knowledge, and fosters new technologies to address critical issues facing Russia and the world.

The Computational Materials Design Lab at Skoltech develops novel methods for computational materials discovery and applies them to a wide range of exciting scientific problems. Under the directorship of Professor Artem Oganov (Center for Energy Science and Technology, Skoltech) and Professor Vladimir Anisimov (Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences), the Lab carries out world-leading research into new materials for application in energy, transport, oil and gas, and other sectors. Established in 2015, the Lab was co-founded by the Gazprom Neft Science & Technology Center.

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Challenge

The computer-aided design of new materials makes it possible to discover previously unknown materials with exceptional properties. By using predictive computational methods, researchers can find superhard, magnetic, thermoelectric, and superconducting materials.

Thanks to AI-powered algorithms, scientists can predict the structure and properties of new compounds faster than through experimentation. This revolutionary field of materials science requires a huge amount of high-performance computing (HPC) resources.

> “Analyzing a structure requires four or five separate calculation stages. Each of these calculation stages consists of around 8,000 small jobs that each take two to four hours to run. With 30 researchers completing dozens of individual calculation stages each month, we need to be able to run many hundreds of thousands of jobs in parallel.”

Professor Artem Oganov
Computational Materials Design Lab, Skoltech

Why Lenovo? Maximum performance for parallelized workloads.

With its existing supercomputer approaching end-of-life, the Computational Materials Design Lab at Skoltech engaged Lenovo to deliver a HPC solution better suited to its highly parallelized workloads.

“We wanted to maximize the number of cores and system performance to support many small parallel jobs,” says Professor Oganov. “Lenovo offered the highest number of computational cores within our budget.”

Working with Lenovo Professional Services, the Lab designed a solution based on high-density Lenovo ThinkSystem SD530 servers and the Lenovo Intelligent Computing Orchestration (LiCO) software stack. With up to two high-core-count Intel® Xeon® Scalable processors per node, up to 56 cores total, the Lenovo ThinkSystem SD530 delivers top performance for parallel workloads in a cost-efficient design.

Building the best system for researchers' needs.

The new system, named 'Oleg', comprises 60 Lenovo ThinkSystem SD530 servers. The servers are clustered together using 10Gbps fabric. Intel® Optane™ Persistent Memory boosts server memory capacity, delivering low-latency, high-throughput storage that enables researchers to process large amounts of data faster than ever.

The Lab worked closely with Lenovo Professional Services to deploy, configure, and fine-tune the cluster to achieve the best performance. With support from Intel® performance application engineers, the Lab optimized its software for multi-core processors, helping to ensure maximum performance for parallelized workloads. And with LiCO software, the Lab gets an easy-to-use graphical interface to deploy, monitor, and manage workloads on the Oleg cluster.

"Support from both the Lenovo Professional Services team and Intel® performance application engineers helped ensure that we get the very best performance from our new cluster."

Professor Artem Oganov
Computational Materials Design Lab, Skoltech

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Results

With the Oleg cluster, researchers at the Computational Materials Design Lab at Skoltech have access to powerful HPC resources that deliver a significant increase in compute performance compared to the previous system, particularly for parallelized workloads. The Lab's scientists can process and analyze data faster and get the results of calculations quicker, cutting time-to-insight.

For example, the Lab is currently exploring high-temperature superconductivity. The structures of some of the highest-temperature superconductors, including thorium hydride and yttrium hydride, were predicted, modeled, and obtained experimentally by the Lab's researchers.

Another team has developed its own program to calculate thermoelectric properties of new materials and have already reported compelling results. They are now working to develop several compounds to study the materials at high-pressure phases, which will help them to refine theoretical predictions in the future.

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Skolkovo Institute of Science and Technology

- **Significant performance increase**
- **Optimized for parallel workloads**
- **Shorter time-to-insight**

“We are constantly working to develop new algorithms to better predict the structure and properties of new materials. Each new generation requires more and more compute resources. With the Lenovo HPC cluster, we have the resources we need to achieve results that we previously considered unattainable.”

Professor Artem Oganov
Computational Materials Design Lab, Skoltech

What will you do with Lenovo HPC solutions?

The Data-Centered drive groundbreaking materials-science research with
Lenovo smarter infrastructure solutions, powered by Intel® Xeon® Scalable processors

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