

LSQUANT becomes a software module of the Apeiron Intelligence platform!

We are excited to announce that **LSQUANT is being incorporated as a dedicated software module within the Apeiron Intelligence platform**, making its powerful large-scale quantum transport capabilities much easier to access and use by researchers and engineers. **LSQUANT** has been developed over more than two decades to enable **linear-scaling quantum transport simulations of realistic materials and devices**, reaching systems containing millions to billions of atoms. Its methodologies address charge, spin and topological transport in complex and disordered materials and have been applied across nanoelectronics, spintronics, quantum materials, thermal transport and emerging quantum technologies.

LSQUANT already combines highly efficient CPU/GPU implementations with interfaces to tools such as **Wannier90 and Kwant**, enabling multiscale workflows that connect electronic-structure calculations with large-scale quantum transport simulations.

From powerful algorithms to an accessible simulation workflow

By integrating LSQUANT into **Apeiron Intelligence**, we aim to remove much of the technical complexity traditionally associated with deploying large-scale quantum-transport simulations. Apeiron's AI-driven scientific platform is designed to help users configure, execute and analyse advanced materials simulations through an integrated computational environment. The combination means that researchers and engineers will increasingly be able to move from a **materials structure or electronic Hamiltonian to experimentally relevant transport properties** without having to become specialists in the underlying HPC implementation.

The objective is simple: **make the extraordinary computational power of LSQUANT available to a much broader scientific and industrial community.**

Through Apeiron, LSQUANT can become part of larger workflows connecting **first-principles calculations, machine-learned Hamiltonians, atomistic modelling and large-scale transport simulations**, opening the possibility of studying realistic materials and devices at previously inaccessible length scales.

Quantum transport at realistic scales. Linear-scaling methodologies fundamentally change the size of systems that can be investigated computationally. LSQUANT was specifically conceived to address quantum transport in complex materials where conventional matrix diagonalisation or inversion methods rapidly become computationally prohibitive.

Its integration into Apeiron therefore represents an important step toward bringing **predictive quantum transport modelling closer to materials discovery, device optimisation and industrial R&D.**

LSQUANT + Apeiron Intelligence: billion-atom quantum simulation made easier to access, automate and connect to the broader materials-modelling workflow.

Discover **Apeiron Intelligence**: <https://www.apeironagents.tech/>