Approved computing time projects on the JARA partition

(period May 01, 2022 - April 30, 2023)

DFG Classification		Project Title	HPC Resource	Name of PI	Institution
2 - Life Sciences	21 - Biology	Molecular dynamics simulations of P2X receptors	CLAIX CPU	Prof. Machtens	Forschungszentrum Jülich
		Molecular dynamics simulations of P2X receptors	CLAIX GPU	Prof. Machtens	Forschungszentrum Jülich
	22 - Medicine	Improved Diagnostics of Respiratory Flows Using a Lattice-Boltzmann Method and Machine Learning Techniques	CLAIX CPU	Dr. Lintermann	Forschungszentrum Jülich
3 - Natural Sciences	31 - Chemistry	Computational studies of reactivities in organic and organometallic transformations	CLAIX CPU	Prof. Schoenebeck	RWTH Aachen University
		Theoretical insights into promising barocaloric materials	CLAIX CPU	Prof. Dronskowski	RWTH Aachen University
	32 - Physics	First-principles investigation of single magnetic nano-skyrmions	CLAIX CPU	Prof. Lounis	Forschungszentrum Jülich
		Topological transport in real materials from ab initio	CLAIX CPU	Prof. Mokrousov	Forschungszentrum Jülich
		Trends for quantum-chemistry based material maps	CLAIX CPU	Prof. Wuttig	RWTH Aachen University
		Nuclear Lattice Simulations	CLAIX CPU	Prof. Meißner	Forschungszentrum Jülich
		Exploration of Federal Computing Infrastructures for the Experiments at the CERN Large Hadron Collider	CLAIX CPU	Prof. Schmidt	RWTH Aachen University
4 - Engineering Sciences	42 - Thermal Engineering / Process Engineering	Parallel Stabilized Finite Element Methods for Aero-, Hemo- and Hydrodynamics	CLAIX CPU	Prof. Behr	RWTH Aachen University
		Parallel Stabilized Finite Element Methods for Aero-, Hemo- and Hydrodynamics	CLAIX GPU	Prof. Behr	RWTH Aachen University
	43 - Materials Science and Engineering	Statistical analysis of highly-nanoporous materials using molecular dynamics and machine learning	CLAIX CPU	Prof. Markert	RWTH Aachen University
	44 - Computer Science, Electrical and System Engineering	Optimizing Wide-Area Network Configurations with Quantum Annealing	JUPSI (D-Wave Quantum Annealer)	Prof. Luu	Forschungszentrum Jülich
		Efficient Hyperparameter Optimization on HPC Systems	JUPSI (D-Wave Quantum Annealer)	Dr. Lintermann	Forschungszentrum Jülich