

Approved computing time projects on the JARA partition

(period November 01, 2022 - October 31, 2023)

DFG Classification		Project Title	HPC Resource	Name of PI	Institution
2 - Life Sciences	201 - Biology	Molecular dynamics of the SLC26 family of ion channels and transporters	CLAIX CPU	Prof. Machtens	Forschungszentrum Jülich
		Molecular dynamics of the SLC26 family of ion channels and transporters	CLAIX GPU	Prof. Machtens	Forschungszentrum Jülich
3 - Natural Sciences	302 - Chemistry	Quantum chemistry of functional chalcogenide for phase-change memories and other applications	CLAIX CPU	Prof. Dronskowski	RWTH Aachen University
		Atomistic modeling of energy materials	CLAIX CPU	Prof. Kowalski	Forschungszentrum Jülich
	307 - Physics	Ab initio exploration of rare earth magnets for spintronics applications	CLAIX CPU	Prof. Blügel	Forschungszentrum Jülich
		First-principles investigation of antiferromagnetic topological spin-textures	CLAIX CPU	Prof. Lounis	Forschungszentrum Jülich
		Many-Body Downfolding for Correlated Entangled Systems	CLAIX CPU	Prof. Pavarini	Forschungszentrum Jülich
		Materials for topological quantum computing from first principles	CLAIX CPU	Prof. Rüßmann	Forschungszentrum Jülich
		Materials for topological quantum computing from first principles	CLAIX GPU	Prof. Rüßmann	Forschungszentrum Jülich
		Cluster-Basis Quantum Monte Carlo Simulations of Two-Dimensional Frustrated Magnets	CLAIX CPU	Prof. Wessel	RWTH Aachen University
		HTC with and code evolution of FLEUR	CLAIX CPU	Prof. Wortmann	Forschungszentrum Jülich
Towards a quantum-chemical map for d-bonded materials	CLAIX CPU	Prof. Wuttig	RWTH Aachen University		
4 - Engineering Sciences	404 - Heat Energy Technology, Fluid Mechanics	Analysis and modeling of multi-scale structures of iso-scalar sets in turbulent flows	JUPSI	Prof. Bode	Forschungszentrum Jülich
		Intrinsic flame instabilities and morphodynamics of turbulent premixed hydrogen flames	JURECA-DC CPU	Prof. Gauding	RWTH Aachen University
		Intrinsic flame instabilities and morphodynamics of turbulent premixed hydrogen flames	JURECA-DC GPU	Prof. Gauding	RWTH Aachen University
	406 - Materials Science	Development of efficient and environmentally friendly LONG distance powertrain for heavy duty trucks and coaches – Project LONGRUN	CLAIX CPU	Prof. Guenther	RWTH Aachen University
		Rational Design of Porous Carbon Anodes for Low Cost Batteries	CLAIX CPU	Prof. Khetan	RWTH Aachen University
		Quantum-mechanical investigations of phase stability, local chemical ordering and defect formation in MAX/MAB phases and compositionally complex multielement systems	CLAIX CPU	Prof. Schneider	RWTH Aachen University