Postdoc on exploring optimal tensor structures for machine-learning potentials

ReferenceNr.: MCL_272

Materials Center Leoben Forschung GmbH (MCL) is a leading competence center in the field of materials research and technology. In this context, we support numerous companies in the production sector developing high-performance materials, manufacturing processes and products. By developing specific computer-aided technologies, we accelerate materials based innovation including the digitalization of the manufacturing chain as well as of products. Our portfolio includes cooperative research and development projects with international and national partners from the production and research sectors as well as several consulting, laboratory and simulation services in materials science.

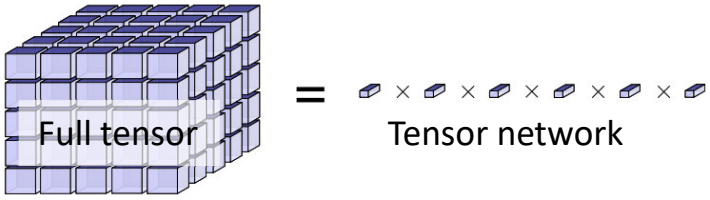
Would you like to work in an innovative and international setting?
Then MCL is the perfect work place for you!

Your Profile

You have—or will shortly receive—a doctoral degree in any of the computational sciences (e.g., computational materials science/physics/chemistry, applied mathematics). The project requires knowledge in

- linear algebra/machine-Learning methods,
- programming (e.g., C/C++, Python),
- crystallography/atomic-scale mechanics,
- atomistic simulation,

and you are enthusiastic about mastering them to develop new AI methods to accelerate the design of innovative materials.



Tasks & Responsibilities

Machine-learning interatomic potentials (MLIPs) have been a breakthrough for providing the quantitative accuracy of quantum mechanics to atomistic simulations. However, they suffer from a very high complexity (e.g., millions of parameters) when applied to systems with a large chemical space, also involving other quantum-mechanical phenomena like magnetism.

In this project, you will explore tensor networks, a way of compressing high-dimensional parameter tensors with several lower-order tensors, as a representation of machine-learned atomic descriptors. The challenge of applying tensor networks to MLIPs are symmetries (e.g., rotational invariance of atomic energies), which need to be preserved by the tensor network. Your main tasks will revolve around advancing compression algorithms to such symmetry-preserving tensor networks.

Our offer:

- flexible working hours
- further training/education
- home office
- employee events
- cooperation with Firmenradl

A permanent employment contract starting from January 2026 and a gross salary per year of € 64.618,40 (40h/week). The above project on which you are being hired is planned for a duration of 2.5 years.

Please send us your application and a detailed resume. We are looking forward to it!
We would like to especially encourage women to apply.

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