



Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

CSElab

Computational Science & Engineering Laboratory

Using High-Performance Uncertainty Quantification Framework to calibrate Interatomic Potentials

Semester Thesis

Noah Andrés Baumann

noabauma@student.ethz.ch

Computational Science & Engineering Laboratory
ETH Zürich

Supervisors:

Ermioni Papadopoulou

Ivica Kičić

Prof. Dr. Petros Koumoutsakos

September 16, 2021