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Stabilized quasi-Newton optimization of noisy potential energy surfaces BASTIAN SCHAEFER, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland, S. ALIREZA GHASEMI, Institute for Advanced Studies in Basic Sciences, P.O. Box 45195-1159, IR-Zanjan, Iran, SHANTANU ROY, STEFAN GOEDECKER, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland, GOEDECKER GROUP TEAM — Optimizations of atomic positions belong to the most frequently performed tasks in electronic structure calculations. Many simulations like global minimum searches or the identification of chemical reaction pathways can require the computation of hundreds or thousands of minimizations or saddle points. To automatize these tasks, optimization algorithms must not only be efficient but also very reliable. Unfortunately, computational noise in forces and energies is inherent to electronic structure codes. This computational noise poses a severe problem to the stability of efficient optimization methods like the limited-memory BroydenFletcherGoldfarbShanno algorithm. In this talk a recently published technique that allows to obtain significant curvature information of noisy potential energy surfaces is presented. This technique was used to construct both, a stabilized quasi-Newton minimization method and a stabilized quasi-Newton saddle finding approach. With the help of benchmarks both theminimizerandthe saddle finding approach were demonstrated to be superior to comparable existing methods.

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