Workflow and data management with ASE

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The Atomic Simulation Environment (ASE) [1] is a Python library containing tools for working with atoms. We will show how to use ASE for storing the results of "precision quantification" calculations in databases and how to work with the data. We will also go through an example showing how to use ASE for doing the actual calculations.

References

[1] A. H. Larsen, J. J. Mortensen, J. Blomqvist, I. E. Castelli, R. Christensen, M. Dulak, J. Friis, M. N. Groves, B. Hammer, C. Hargus, E. D. Hermes, P. C. Jennings, P. B. Jensen, K. Kaasbjerg, J. Kermode, J. R. Kitchin, E. L. Kolsbjerg, J. Kubal, S. Lysgaard, J. B. Maronsson, T. Maxson, T. Olsen, L. Pastewka, A. Peterson, C. Rostgaard, J. Schitz, O. Schtt, M. Strange, K. Thygesen, T. Vegge, L. Vilhelmsen, M. Walter, Z. Zeng, and K. W. Jacobsen, J. Phys.: Condens. Matter **29** 273002 (2017)