O.5 Atomic Simulation Recipes for automated workflows: Application to 2D materials

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In this talk will introduce the Atomic Simulation Recipes (ASR) – a new open source Python framework for working with atomistic materials simulations in an efficient and sustainable way that is ideally suited for high-throughput studies[1]. Central to ASR is the concept of a Recipe: a high-level Python script that performs a well-defined simulation task robustly and accurately while automatically keeping track of the data provenance. Being independent objects with automatic data provenance logging, Recipes may be freely combined through Python scripting giving maximal freedom for users to build advanced workflows that can be executed using workflow managers like the MyQueue task scheduler[2]. The ASR leverages the functionalities of the Atomic Simulation Environment (ASE)[3] to interface with external simulation codes, attain a high abstraction level, and create databases that may be easily presented as web pages. I will give examples on the use of ASR for high-throughput computations in the context of 2D materials research [4].

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[1] https://psi-k.net/download/highlights/Highlight_151.pdf

[2] MyQueue: Task and workflow scheduling system, Mortensen et al., 2020 Journal of Open Source Software, 5(45), 1844, https://doi.org/10.21105/joss.01844

[3] The atomic simulation environment – a Python library for working with atoms, Larsen et al., 2017 J. Phys.: Condens. Matter, 29, 273002, https://doi.org/10.1088/1361-648X/aa680e

[4] The Computational 2D Materials Database: High-Throughput Modeling and Discovery of Atomically Thin Crystals, S. Haastrup et al., 2D Materials 5, 042002 (2018)