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Automated Workflows and Machine Learning for Materials Science Simulations

Machine learning techniques in physics and materials science have revolutionized simulations and experimental analysis. Using these techniques to accurately predict, for example, material properties requires the manipulation and use of vast amounts of data. Manual processing and analysis quickly become impractical and error-prone, so the availability of automated workflows is critical to their efficient, reliable, and consistent application. In this tool-demo, we provide an practical introduction to workflow management using Pyiron (www.pyiron.org). Pyiron is an integrated materials science development environment based on Python and Jupyter notebooks that can be used for a wide range of simulation tasks, including rapid prototyping, coupling with experiments, and high-performance computing. The demo gives a general introduction to the use of Pyiron with a focus on atomistic simulation tasks. As a practical example, the relevant steps of the workflow for the construction of ab initio phase diagrams will be demonstrated, with the focus on the training and validation of machine learning potentials that are used for this purpose.

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