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the vienna ab initio simulation package atomic scale materials modelling from first principles [read more](#)

requests for technical support from the vasp team should be posted in the vasp forum

install vasp and find the tutorial that suits you you will need the vasp executable in your system path and a working directory in which you run the tutorials

about what is vasp the vienna ab initio simulation package vasp is a computer program for atomic scale materials modelling e g electronic structure calculations and quantum mechanical

analyze vasp output the output files written by vasp depends on the kind of calculation you are running py4vasp is the most seamless tool to extract data from vasp calculations it is a python

step 1 download download the source code of vasp from the vasp portal copy it to the desired location on your machine and unzip the file to obtain the folder path to vasp x x

x and reveal its

tutorials new to vasp with our detailed tutorials you can learn to run your vasp calculations

vasp looks in the current directory for four main input files i e poscar incar kpoints and potcar the general format of each input file is explained in details in the linked articles that lead

about what is vasp and what can i do with it get a brief overview of the method and a list of the features

Jul 15 2025 we invite you to participate in the first vasp workshop of the year three days on nuclei and core electrons in vasp getting close to the nucleus you will be introduced to vasp and

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