

Vienna Ab Initio Simulation Package Source Code Free Download



The Vienna Ab initio Simulation Package, better known as VASP, is a package for performing ab initio quantum mechanical calculations using either Vanderbilt, or the Gaussian method. In the case of the Gaussian method, it relies on the possibility of applying a technique known as the Gaussian-Wu Jing method, which uses a quantum mechanical approach. In the case of Vanderbilt, the quantum mechanical approach relies on Wigner's mass conservation theorem. This method uses a method to solve the Schrödinger equation, which can be solved in two ways: quantum mechanical or numerical integration.

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