

In this blog post, I'm going to show you how to cite VASP in your scientific research articles. Recently, I was working with VASP and then needed to put the results in a manuscript. So, I needed to cite it, and that prompted me to research a bit.

Why Citing VASP Matters

When you use VASP (Vienna Ab initio Simulation Package) in your research, it's important to credit the developers. Citing VASP helps others understand your methods and ensures reproducibility. It also recognizes the extensive work behind the tool.

Key Papers to Cite

VASP has several key papers that cover different aspects of its development. Depending on your work, you may need to reference one or more of the following:

1. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set
Physical Review B, 1996
Authors: Georg Kresse, Jürgen Furthmüller
[Link to paper](#)
2. From ultrasoft pseudopotentials to the projector augmented-wave method
Physical Review B, 1999
Authors: Georg Kresse, Daniel Joubert
[Link to paper](#)
3. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set
Computational Materials Science, 1996
Authors: Georg Kresse, Jürgen Furthmüller
[Link to paper](#)
4. Ab initio molecular dynamics for liquid metals
Physical Review B, 1993
Authors: Georg Kresse, Jürgen Hafner
[Link to paper](#)
5. Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium
Physical Review B, 1994
Authors: Georg Kresse, Jürgen Hafner
[Link to paper](#)
6. Norm-conserving and ultrasoft pseudopotentials for first-row and transition elements
Journal of Physics: Condensed Matter, 1994
Authors: Georg Kresse, Jürgen Hafner
[Link to paper](#)

Citation Formats and Tools

Citing scientific tools can be tedious. To make it easier, you can use citation files. Here are the formats and where to download them:

- EndNote (.enw): [Download .enw file](#)
- RIS (.ris): [Download .ris file](#)
- BibTeX (.bib): [Download .bib file](#)
- CSV (.csv): [Download .csv file](#)

You can use these files with tools like EndNote, Zotero, or LaTeX. For instance, in LaTeX, you can include the BibTeX

```
@article{kresse1996,  
  title={Efficient iterative schemes for ab initio total-energy calculations using a  
plane-wave basis set},  
  author={Kresse, Georg and Furthmüller, Jürgen},  
  journal={Physical Review B},  
  volume={54},  
  pages={11169- -11186},  
  year={1996},  
  publisher={APS}  
}
```

Watch the Video

For a step-by-step guide, watch my YouTube video where I demonstrate how to download and use these citation files:

Final Thoughts

Citing VASP correctly shows professionalism and supports the scientific community. It's a small effort that makes a big difference in research integrity. If you have questions, feel free to leave a comment below or on the YouTube video.



Manas Sharma

I'm a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, and Machine Learning related apps and software from time to time. Can code in most of the popular languages. I like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

manas.bragitoff.com/

Share this:

Click to share on Facebook (Opens in new window)

Click to share on Twitter (Opens in new window)

Click to share on WhatsApp (Opens in new window)

Click to share on Pinterest (Opens in new window)

Click to share on Reddit (Opens in new window)

Click to share on LinkedIn (Opens in new window)

Click to email a link to a friend (Opens in new window)

Click to print (Opens in new window)

Click to share on Tumblr (Opens in new window)

Click to share on Pocket (Opens in new window)

Click to share on Telegram (Opens in new window)

[wpdon id="7041" align="center"]