

# **“Why the hell did you not use VASP?” Pros and cons of ABINIT in the high-throughput world**

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High-throughput computation is an emerging area of ab initio materials design. The vast majority of high-throughput computations have been performed using VASP but the use of other plane-wave codes such as ABINIT is currently growing. A case in point is the recent building of a high-throughput phonon database using ABINIT and DFPT.

We will provide a personal view from a materials designer/user perspective on the pros and cons from different plane wave codes and especially VASP (with possible additional wrappers such as phonopy) and ABINIT. I will focus on current activities in our group targeting the use of ABINIT especially for linear and non-linear response computations (phonons, electron-phonon, non-linear optics). This general overview talk will be followed by more detailed and technical talks. It will hopefully motivate further discussion on the priority in ABINIT future developments as an additional engine to high-throughput computational design.