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APPROX. METHOD AND SOFTWARE

The approximation methods used are

- LDA (Local Density Approximation)
- LSDA (Local Spin Density Approximation)
- GGA (Generalized Gradient Approximation)
- The Xa Method (Hartree-Fock-Slater method)
- Meta-GGA Functionals
- Hybrid GGA

The software which is most popular in calculating DFT is the

VASP (Vienna Ab initio Simulation Package)



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