Implementing the Relaxed Core PAW Method into ABINIT

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20.05.2019

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- However in extreme conditions, like warm dense matter or high pressures, core energies are known to change considerably.
- Especially under warm dense matter conditions, the cost of using all-electron codes is to high.
- Therefore an intermediate method is necessary.

Model and Implementation

Relaxed Core PAW

- Method proposed by Marsman and Kresse [a]
- General idea, relax cores in between SCF cycles:
  - Solve atomic problem with fixed (DFT) valence charge density to obtain new AE core density.
  - Calculate new core AE partial waves.
  - Calculate new PS partial waves, that remain dual to the original projectors.
  - Recalculate dependent parameters.

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- We will modify the pawtab data structure in an unobtrusive way (e. g. pointers) to allow for changes.

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- Use Vanderbilt method to allow for unmodified projectors.
- Recalculate D_{ij} and Q_{ij}.
- Introduce suitable mixing.
- Resume SCF cycle.

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- For many applications one relaxed atom might be sufficient.
- However, if all atoms should be relaxed, a more efficient approach might be necessary, e. g. separate again between per atom and per atom-type data.
- Downside: More coding and more potential for unexpected interactions with the rest of ABINIT.