Capabilities of CP2K with the SIRIUS engime

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Functionalities of CP2K

- CP2K uses the gaussian and planewaves functions as basis set, making it particularly efficient for studying molecules or 3D structures for instance.
- It supports many type of simulations
  - molecular dynamics,
  - structure relaxation,
  - montecarlo simulations,
  - etc... (see http://www.cp2k.org for more details).
- although possible, studying crystaline structures with CP2K is not very easy.
- available on daint both CPU and GPU (no SIRIUS support)

CP2K is actively developed with extensive unit tests and new features are added every month.

CP2K with the SIRIUS engine adds extra functionalities

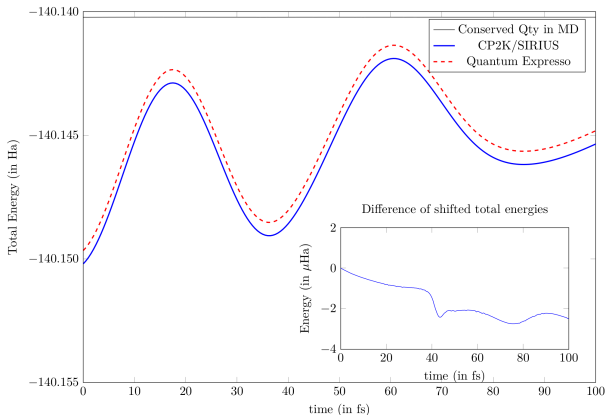Periodic structures are often better described in the planewave domain.

- natively support GPUs, MPI, OpenMP, RoCm (experimental)
- has a python interface
- Use symmetries when possible (or asked)
- Supports many XC (libxc support) and vdw functionals
- Supports, many pseudo-potential (norn conserving, ultra soft, paw) and full potential flavors
- spin-orbit coupling, colinear and non colinear magnetism
- on-site Hubbard correction.
- Is fully integrated to CP2K (when compiled with the support on).
- Only computes the ground state, force and stresses.

Si$_7$Ge relaxation with CP2K/SIRIUS

This cell has nothing special. It is toy model we use for comparison.

We do molecular dynamics at finite T : Protocol

- We do the computation with CP2K / SIRIUS on a $2 \times 2 \times 2$ k-points grid. CP2K returns the atoms coordinates as well as the ground state energy.

- For comparison we use Quantum Expresso (which also supports SIRIUS)

- Use QE for calculating the ground state energy using the atoms coordinates generated by CP2K/SIRIUS

- input files can be found on the C2PK website.

Note the energy shift between QS and CP2K. When corrected the energy difference between QE and CP2K/SIRIUS is in the μHa

Conclusion

- Inclusion of SIRIUS in CP2K provides functionalities only present in Quantum Expresso so far in a single package.
- SIRIUS adds extra functionalities that are not present in QE or CP2K (full potential methods)
- CP2K can be found on daint (apparently without SIRIUS support)
- Please visit http://www.cp2k.org for more details