A GPU-accelerated implementation of DFTB+

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The requirement of accelerating calculations of complex chemical systems, i.e. molecular dynamics in the microsecond time scale, finds an answer in the use of GPUs. Here, a GPU-accelerated implementation of the software DFTB+ [1] is presented. The most-time consuming parts of the code are properly identified and ported to run on GPUs. Several benchmark calculations are carried out to assess the speed-up of the code, which show that the full potential and acceleration of the GPUs is only reached when the size of problem is large enough (matrices larger than 6000×6000).

References

1. B. Aradi, B. Hourahine, and Th. Frauenheim, *J. Phys. Chem. A*, **111** 5678 (2007).