Recently updates of DCDFTBMD program: Theory, implementation, and applications

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Our research group has developed the massively parallel DCDFTBMD program [1], which combines the divide-and-conquer type density-functional tight-binding (DC-DFTB) method [2] with the molecular dynamics (MD) simulation technique in the last decade. The original motivation of the development was the filling the big gap in sizes treated by the classical and quantum MD simulations. For this, we have focused on implementing the DC-DFTB energy and its derivatives with high efficiency [2,3] and supporting a variety of simulation methods [1,4]. We here introduce some of the recent updates in the DCDFTBMD program. The presentation first covers performance evaluation of the code on the Fugaku supercomputer, one of the most advanced computers in the world. The demostrative calculations of 50–100 million atoms was achieved by overcoming a memory bottleneck with direct self-consistent charge-like algorithm [5]. We next explains the development of the species-selective nanoreactor MD technique [6], which can accelerate the chemical reactions ofcomplex systems in solution under relatively mild conditions. Finally, several applications of the DCDFTBMD programs are introduced, for example, materials and bio systems.

References

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