Self-consistent Field Theory for Nanostructure Discovery

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Block copolymer self-assembly is a versatile building block for nanostructure design and fabrication in many applications. The explanatory simulation approach to study this phenomenon is self-consistent mean field theory (SCFT). It is a well-developed formalism to discover thermodynamically stable states in self-assemblies systematically. However, as the architecture of block copolymers in experiments becomes complicated for designing various nanodevices, the computational power requirement in SCFT is raised to discover new but complex order states. In this contribution, we carefully validate the symmetric as well as asymmetric phase diagram of di-block copolymer system by an in-house GPU platform. Our results demonstrate that the platform constructs phase diagrams up to 30 times faster than traditional CPU-based implementations. Furthermore, we successfully identify complex spherical and network phases such as the Frank–Kasper σ phase [1] and the Fddd (O^{70}) phase [2], which have been observed experimentally for some time but have only recently been confirmed as stable phases through theoretical calculations. We anticipate that this framework can be extended to more intricate block copolymer architectures, thereby accelerating the discovery of novel stable phases through high-performance computation.

References

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