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Practical Boundary Conditions for Electronic Structure Calculations

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Computational materials design is an active area of research which aims at predicting physical and chemical properties of various materials from first-principles electronic structure calculations. To keep the computational costs manageable, the Schrödinger equations are often approximated by Kohn-Sham equations within the framework of density-functional theory [1]. These Kohn-Sham equations are solved numerically either by a basis set expansion or real-space discretization under given boundary conditions. In the case of a plane-wave basis set, it is common practice to apply periodic boundary conditions in all directions [1], while isolated boundary conditions are more common for the atomic basis set. However, there are many other options besides these standard boundary conditions. In this talk, we will explore several non-standard boundary conditions which exploit the characteristics of each system, such as surfaces, interfaces, and cyclic/helical structures, to minimize the computational costs of electronic structure calculations. Most of these boundary conditions are easily implemented by minor modifications of existing electronic structure codes. Numerical examples on a few model systems are also presented for the validation of these boundary conditions.

REFERENCES

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