Implementation of Periodic Boundary Conditions for the General GFN Force-Field

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We present an implementation of periodic boundary conditions into the general force-field GFN-FF [1]. GFN-FF is designed for fast geometry optimizations and molecular dynamic simulations for large systems, showing excellent performance for various (bio)chemical systems including (transition)metal complexes and related compounds. It is parametrized for all elements up to Radon, which makes it a versatile tool for a large variety of applications. The addition of periodic boundary conditions enables the routine calculation of solid state systems, increasing its general applicability.
This initial work explains the steps that have to be taken to make GFN-FF applicable to solids and molecular crystals. Because the potential contains some non-standard terms, the implementation is rather involved. The electrostatic interactions are calculated with an electronegativity equilibrium (EEQ) model[2] and Ewald summation. Dispersion is calculated using a modified version of the D4 scheme [3]. For validation, we present preliminary tests on the X23 benchmark [4], which show promising results of the periodic implementation.

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