



## Periodic boundary conditions

PySCF supports [electronic structure calculations of extended systems with periodic boundary conditions \(PBCs\)](#). PBC-specific functionality must be imported from `pyscf.pbc` [[../pyscf\\_api\\_docs/pyscf.pbc.html#module-pyscf.pbc](#)], which has a directory structure that mirrors that of the molecular `pyscf` [[../pyscf\\_api\\_docs/pyscf.html#module-pyscf](#)] module, e.g. `from pyscf.pbc import gto, scf`. Details of how to specify the system details, including the unit cell, basis sets, and pseudopotentials, are provided in [Crystal structure](#) [[pbc/gto.html#user-pbc-gto](#)].

All electronic structure methods can be applied with periodic boundary conditions at the Gamma point of the Brillouin zone,  $k = (0, 0, 0)$ , as described in [Mixing PBC and molecular modules](#) [[pbc/mix\\_mol.html#mix-mol](#)]. Converging to the thermodynamic limit requires the use of larger and larger supercells, which might quickly become prohibitive.

More affordable convergence to the thermodynamic limit can be obtained with the use of k-point sampling. A calculation performed with a unit cell and multiple uniformly distributed k-points is equivalent to one performed with a supercell and a single k-point, but is significantly more affordable due to the explicitly enforced translational symmetry (leading to crystal momentum conservation). Only a subset of all methods in PySCF support k-point sampling and they are prefixed with “K”, e.g., KHF, KCCSD, etc.

[Crystal structure](#) [[pbc/gto.html](#)]

[SCF and DFT methods](#) [[pbc/scf.html](#)]

[Density fitting for crystalline calculations](#) [[pbc/df.html](#)]

[Mixing PBC and molecular modules \[pbc/mix\\_mol.html\]](#)