# QCTFF: On the Construction of a Novel Protein Force Field

In this perspective, we explain the strategy behind QCTFF, the current name for a novel atomistic protein force field. The atoms are constructed using Quantum Chemical Topology (QCT). These topological atoms determine how a system's energy is partitioned. We give a brief account of the results hitherto obtained, and a glimpse of unpublished results. Combining this QCT partitioning with the universal quantum expression of energy, leads to four types of fundamental energy contributions. The first of these is intra-atomic and the remaining three interatomic: (i) atomic self-energy, (ii) Coulomb energy, (iii) exchange energy, and (iv) correlation energy. All structural and dynamic effects emerge from the interplay of these contributions. The machine learning method kriging captures well how they change in response to a change in nuclear configuration. Second, the Coulomb energy is represented by a converging multipolar series expansion when the nuclei are sufficiently far apart.

**Reference:**

Paul Popelier, Internat. J. Quant. Chem., DOI: 10.1002/qua.24900, Early View (2015)