

Quantum similarity and molecular alignments with *ab initio* accuracy

Laszlo Fusti-Molnar PhD, QTP

Abstract

Molecular quantum similarities and our new accurate and efficient molecular alignment method will be presented based on first principle electronic structure calculations. This new scheme maximizes quantum similarity matrixes in the relative orientation of the molecules and uses Fourier transform techniques for two purposes. First, building up the numerical representation of true *ab initio* electronic densities and their Coulomb potentials are accelerated by the previously described Fourier Transform Coulomb method. Second, the Fourier convolution technique is applied for accelerating optimizations in the translational coordinates. In order to avoid any interpolation error, the necessary analytical formulae are derived for transformation of the *ab initio* wavefunctions in rotational coordinates. The results of our first implementation for a small test set is analyzed in details and compared with published results of the literature. This new alignment technique is generally applicable for overlap, Coulomb, kinetic energy etc. quantum similarity measures and can be extended to a genuine docking solution with *ab initio* scoring.