MS36 Software development in quantum mechanics-based methods of crystallography

MS36-03

DiSCaMB - a package for computations with aspherical atom form factors (HAR, TAAM)

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Abstract

DiSCaMB is a C++ library (python interface is also planned) for performing crystallographic calculations related to atomic form factors. It is accompanied by programs which both exemplifies use of the library and can be applied in real life crystallographic calculations – for example to generate (*.tsc) file [1,2] with atomic form factors which can be subsequently use for refinement with e.g. Olex2[3]. DiSCaMB provides functionalities related to models used in quantum crystallography such as Hirshfeld Atom Refinement (HAR) and to Transferable Aspherical Atom Model (TAAM).

Atomic form factors in HAR are based on atomic densities obtained by partition of electron density derived from wave function calculations. TAAM relies on transferability of atomic densities between atoms in similar chemical environments. TAAM implementations uses banks of atomic density parameters (e.g. Invariom [4], ELMAM2 [5], MATTS – successor of UBDB [6](which is used by DiSCaMB), etc.)). The densities are expressed in terms of Hansen-Coppens[7] multipole model. DiSCaMB includes tools for performing all of the intermediate step from acquiring information about crystallographic structure to obtaining atomic form factors (see Fig.1).

Since its public release [8] which have had rather limited functionality, DiSCaMB developed into a software for exploring new approaches in quantum crystallography, including application of alternative electron density partitions in HAR [9], speeding up HAR with fragmentation and testing its relation to TAAM [10] and applying TAAM approach including a refinement against X-ray [11] and electron [12] scattering data.

Here we present full spectrum of DiSCaMB capabilities which will be available with the upcoming major new release of the library.

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Fig. 1. Some of DiSCaMB functionalities.