

RMCPProfile7: Reverse Monte Carlo program for modelling of multiphase systems

Wojciech A. Slawinski, Helen Y. Playford

It is increasingly recognised that understanding material structure across a range of length scales is vital for the understanding of material properties. Functional materials are becoming more and more complex, and the use of *in situ* and *in operando* measurements are often required to understand them, leading to the use of more complicated sample environment during measurements. Therefore, the implementation of multiple phase modelling to the RMCPProfile program was considered a necessary development. In this talk I will present RMCPProfile7: a version of RMCPProfile for the modelling of multiphase data, which has a completely rewritten and modernised Fortran codebase. Plenty of novel functionalities such as variety of data types, multiples of datasets, a number of molecular potential restraints, complex rigid body move types (translation, rotation and swap), multiple atom swapping compatible with other restraints, extended program output and log, and many other small-but-useful options have been introduced.