O.1 Software strategy and goals of the Center of Excellence TREX – Targeting Real chemical accuracy at the EXascale

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I will present here the software development strategy and current achievements of the new CoE TREX "Targeting Real chemical accuracy at the EXascale", which has commenced its activities on 1 October 2020. TREX focus is the development and application of stochastic quantum Monte Carlo (QMC) methods. This methodology encompasses various techniques at the high-end in the accuracy ladder of electronic structure approaches and is uniquely positioned to fully exploit the massive parallelism of upcoming exascale architectures.

TREX main objective is to develop a user-friendly and open-source software suite, which integrates TREX codes in an inter-operable and high-performance platform. Core of our software efforts will be the creation of a QMC kernel library (QMCkl) for high-performance QMC simulations and an I/O library for exchanging information among TREX codes.