

entos: A quantum molecular simulation package

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entos is designed for *ab initio* MD simulations of molecular and condensed-phase chemical reactions and other processes, with particular focus on mean-field and quantum embedding methods for electronic structure. The *entos* software package is developed in the C++14 programming language with a structure that enables flexibility (by providing a long-term sustainable platform for development of methods in this area), efficiency (via task-based multi-threaded parallelism), and rigorous software engineering standards.

I. SUMMARY

entos is a software package that enables *ab initio* molecular dynamics calculations on molecular and condensed-phase chemical reactions and other processes. *entos* focuses on multiscale embedding methods that allow for accurate simulation of a small, chemically important region, in a larger, complex chemical environment. Key features include efficient implementations of density-functional theory (DFT),^{1,2} density-corrected DFT,³ embedded mean-field theory (EMFT),⁴⁻⁷ and Grimme's semi-empirical tight-binding method GFN-xTB.⁸ For all of these methods, energy, gradient and semi-analytic Hessian calculations are available. For DFT and EMFT, excited-state calculations are possible through linear response and Δ SCF. All methods support calculations on fractional particle number and fractional spin systems. QM/MM calculations are made possible via combination with external molecular dynamics packages. Classical and quantized molecular dynamics simulations (via ring-polymer molecular dynamics⁹) can be performed with any available energy method.

entos is developed in the C++14 programming language with a clear and well-designed structure. The design aims included flexibility (in the sense of providing a long-term sustainable platform for development of methods in this area), efficiency (which is realized through a task-based parallelism model), and software engineering standards geared towards industrial use. Parallelism is achieved using the Intel Threaded Building Blocks library.¹⁰ The code has been developed using modern software engineering best practices, including version control, unit testing, test coverage analysis, and continuous integration.

Public release of *entos* is scheduled for calendar year 2019.

II. ACKNOWLEDGEMENTS

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