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 ΔSCF. 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 dynamics[9]) 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

We gratefully acknowledge financial support from: the Engineering and Physical Sciences Research Council (EPSRC) (grants EP/M013111/1, EP/P022308/1, EP/R011656/1, EP/R014493/1); the EPSRC Centre for Doctoral Training in Theory and Modeling in the Chemical Sciences (EP/L015722/1); the Royal Society Newton International Fellowship programme; the U.S. Department of Energy (DE-FOA-0001912); the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award No. DE-SC0004993; the Caltech Resnick Sustainability Institute, The Dow Chemical Company, and Toyota Central R&D Labs, Inc.

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