Atomistic-scale simulations of realistic - messy, nasty and complex - reactive materials: the ReaxFF reactive force field and its applications.

Adri van Duin[1]

[1]*Department of Mechanical Engineering, Penn State, University Park PA 16802, USA*

ABSTRACT

The ReaxFF method provides a highly transferable simulation method for atomistic scale simulations on chemical reactions at the nanosecond and nanometer scale. It combines concepts of bond-order based potentials with a polarizable charge distribution.

Since it initial development for hydrocarbons in 2001[1], we have found that this concept is transferable to applications to elements all across the periodic table, including all first row elements, metals, ceramics and ionic materials[2]. For all these elements and associated materials we have demonstrated that ReaxFF can accurately reproduce quantum mechanics-based structures, reaction energies and reaction barriers, enabling the method to predict reaction kinetics in complicated, multi-material environments at a relatively modest computational expense. At this moment, over 1000 publications including ReaxFF development of applications have appeared in open literature and the ReaxFF code – as implemented in LAMMPS, ADF, or in standalone-format – has been distributed to over 1500 academic and industrial groups around the world.

This presentation will describe the current concepts of the ReaxFF method, the current status of the various ReaxFF codes, including parallel implementations and acceleration methods. Also, we will present and overview of recent applications to a range of materials of increasing complexity, with applications to combustion, high-energy materials, ferroelectric materials, catalysis, 2D-materials, aqueous phase chemistry and material failure. For all these applications, we will show how ReaxFF allows us to perform simulations that approach the experimental material complexity.

References

[1] van Duin, A. C. T., Dasgupta, S., Lorant, F., and Goddard, W. A., 2001. ReaxFF: A reactive force field for hydrocarbons. Journal of Physical Chemistry A 105, 9396-9409.

[2] Senftle, T., Hong, S., Islam, M., Kylasa, S.B., Zheng, Y., Shin, Y.K., Junkermeier, C., Engel-Herbert, R., Janik, M., Aktulga, H.M., Verstraelen, T., Grama, A.Y. and van Duin, A.C.T. (2016) The ReaxFF Reactive Force-field: Development, Applications, and Future Directions. Nature Computational Materials 2, 15011.

Adri van Duin Bio.

- Undergraduate degree from University of Amsterdam (1991, Chemistry with Chemical Engineering focus)
- PhD degree from Delft University of Technology 1997 - Chemistry, with organic geochemistry (oil formation) focus
- Worked from 1997-2002 at the University of Newcastle upon Tyne - molecular dynamics simulations on wettability and
phase partitioning related to oil migration.
- Awarded Marie Curie and Royal Society Fellowships in Newcastle
- 1999-2001: Invented the ReaxFF method - in collaboration with prof. Goddard's group at Caltech
- In 2002 joined prof. Bill Goddard's group at Caltech as the Director of Force Field Simulations
- 2008: Joins the Department of Mechanical and Nuclear Engineering at Penn State as Associate Professor
- Fall 2013: co-founder and CTO of RxFF_Consulting, a company that consults for the development and application of ReaxFF force fields.
- Fall 2014: Courtesy appointment as Associate Professor in Chemical Engineering at Penn State
- January 2015: Director of Material Computation Center at Penn State
- January 2015: Awarded Kenneth Kuan-Yun Kuo Early-Career Professorship
- Spring 2015: Promoted to Professor
- Spring 2016: Courtesy appointment as Professor in Engineering Science and Mechanics at Penn State
- Spring 2018: Courtesy appointment as Professor in Chemistry at Penn State
- Spring 2018: Courtesy appointment as Professor in Material Science and Engineering at Penn State

Currently leads a research group of around 25 people – 15 PhD students and 10 postdoctoral scientists.

Inventor and main developer of the ReaxFF reactive force field method - has published over 450 journal papers (over 400 ReaxFF related) and has distributed the ReaxFF code to over 2500 university and industrial research groups all over the world. Developed a graduate course (ME/ChE 597) introducing atomistic-scale simulations to engineers.
Research focus: Atomistic-scale simulations on complex, dynamics, chemically reactive materials, molecules and interfaces.