Newark College of Engineering

Presents

Adri van Duin

Series Seminar for Engineering Students and Faculty
April 19, 2021 at 4:00 p.m. via WebEx

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

Speaker: Adri van Duin, Penn State University

Adri van Duin's research focuses on Atomistic-scale simulations on complex dynamics, chemically reactive materials, molecules and interfaces. Mr. van Duin is inventor and main developer of the ReaxFF reactive force field and is co-founder and CTO of RxFF Consulting. He 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. Mr. van Duin has an Undergraduate degree in Chemistry from University of Amsterdam, focusing in Chemical Engineering and a PhD degree in Chemistry from Delft University of Technology.

Mr. van Duin has been with the Department of Mechanical and Nuclear Engineering at Penn State since 2008 and holds Courtesy Appointments in Chemical Engineering, Engineering Science and Mechanics, Chemistry, and Materials Science and Engineering. He is Director of the Materials Computation Center and was recently promoted to Distinguished University Professor. He currently leads a research group of 15 PhD students and 10 postdoctoral scientists.

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 its initial development for hydrocarbons in 2001, 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. 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.

To attend this seminar please click here and enter the password as pfWZBmYp393.

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