

Progress in the Industrial Deployment of Materials Modelling Software

Introduction

This session will address the present status of industrial deployment of materials modelling software especially in Europe. Examples of both successful implementations of atomistic simulations in industrial contexts and the barriers to overcome will be discussed. We will also focus on measures to be taken by all stakeholders to promote the integration of materials modelling in industrial processes.

Objectives

- The key objective of this session is an assessment of the progress of the industrial deployment of materials modelling software.
- Related objectives are
 - An understanding of the main drivers of this progress
 - A comparison of the European, American, and Asian companies in terms of the deployment of materials modelling software
 - Assessment of the impact of different business models
- Recommendations to promote the uptake of materials modelling by industry

Background information and documents

The progress in the industrial deployment of materials modelling can be seen from trends such as the number of industrial patents citing materials modelling and the growth in the number of employees being hired in modelling groups.

A series of workshops organized by the University of Vienna “Theory Meets Industry” illustrates global trends and the growing interest of industrial R&D laboratories in materials modelling and simulations. A summary of such a workshop was published in the J. Phys.: Condens. Matter 20 (2008) 064243. At that workshop, Toyota, General Motors and Ford were present showing their materials modelling activities while European car manufacturers were absent.

Together with DuPont in the USA and Sumitomo Chemical in Japan, BASF is one of leaders in the industrial deployment of quantum chemical methods. DuPont installed a supercomputer in 1985 and a few years later Sumitomo Chemical inaugurated its supercomputer. At that time, BASF pioneered the use of quantum chemical calculations on workstation clusters. A milestone in the industrial deployment of materials modelling was the installation of a supercomputer at BASF in 2017, clearly demonstrating the growing relevance of computational modelling in industry.

<https://www.basf.com/global/en/who-we-are/innovation/our-way-to-innovations/supercomputer.html>

Further information on the current industrial deployment of materials modelling can be found on the websites of the leading software providers.

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Additional articles related to this subject are:

Erich Wimmer, Reza Najafabadi, George A Young, Jake D Ballard, Thomas M Angeliu, James Vollmer, James J Chambers, Hiroaki Niimi, Judy Shaw, Clive Freeman, Mikael Christensen, Walter Wolf and Paul Saxe, *Ab initio calculations for industrial materials engineering: successes and challenges*, J. Phys.: Condens. Matter 22 (2010) 384215.

Volker Eyert, Mikael Christensen, Walter Wolf, David Reith, Alexander Mavromaras, Clive Freeman, and Erich Wimmer, *Unravelling the Potential of Density Functional Theory through Integrated Computational Environments: Recent Applications of the Vienna Ab Initio Simulation Package in the MedeA® Software*, Computation 6, 63 (2018)
doi:10.3390/computation6040063.

Discussion points and questions

The following questions summarize the issues for this session.

- Deployment of materials modelling in different industrial sectors including automotive & aerospace, chemical & petrochemical, electronics, specialty materials, pharmaceutical
- What are the main drivers of industrial uptake of materials modelling?
- What type of software is being used and most effective?
- International comparison
- Software as a service
- Organizational aspects, e.g. central modelling groups, modelling embedded in business units, budget, staffing

Expected outcome

- A report describing the information gathered in this workshop session
- The report will provide answers to the following questions:
 - What progress has been achieved during the past decades?
 - Which measures should be taken to increase the uptake of materials modelling in industry?
 - How does the investment in materials modelling in European industry compare with American and Asian companies?