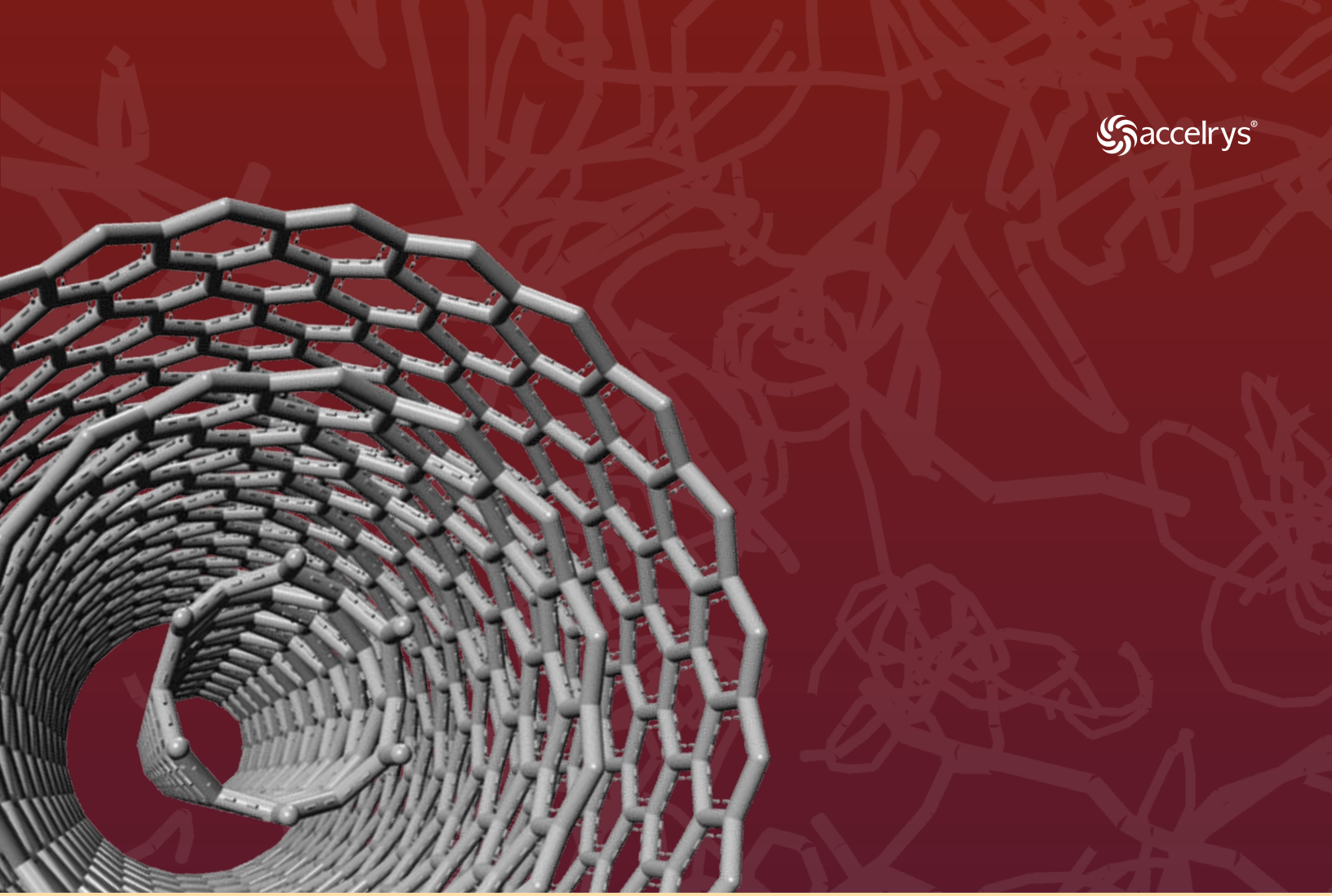


Accelrys Nanotechnology Consortium

Computer Aided Nanodesign™
Software tools to enable the rational design of nanomaterials and nanodevices

Executive Summary

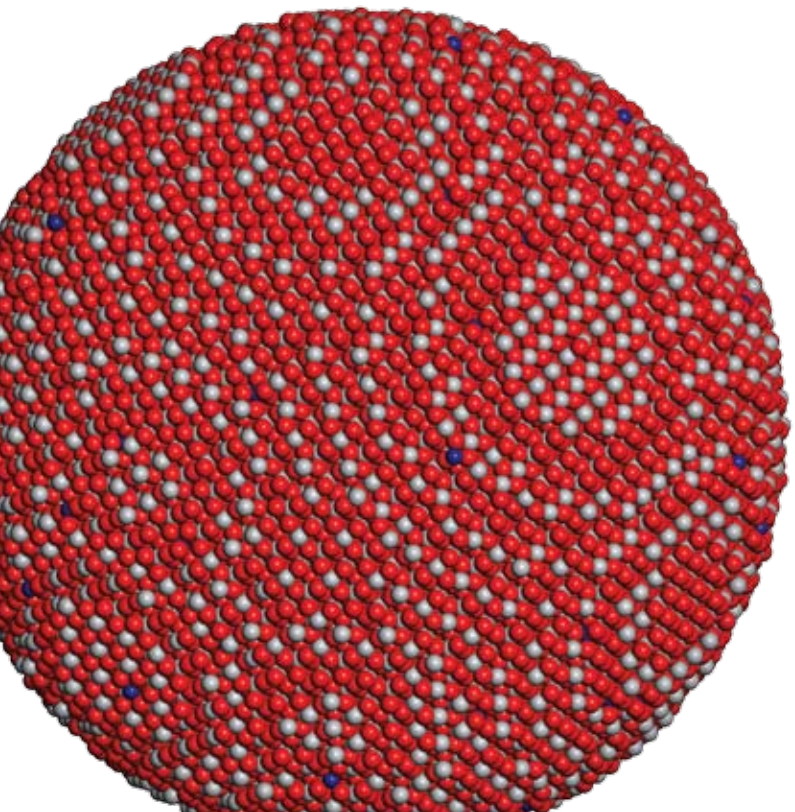
With investment in nanotechnology research in the billions and global competition growing, organizations face increasing pressure to strategically and rapidly apply nanotechnology within their research and development processes. But, today's research in advanced materials and nanotechnology poses unique challenges at the atomistic and molecular scale. Recognizing the potential of software technology to bear strongly upon these challenges, Accelrys, its scientific advisors and customers joined together to form the Accelrys Nanotechnology Consortium in July 2004.

The Consortium gives members the opportunity to work in collaboration with scientific thought-leaders to steer Accelrys' development of leading-edge modeling and simulation software technology. It aims to directly address members' needs to rationally design nanomaterials and nanodevices for applications ranging from the design of catalysts, coatings and adhesives to new materials for electronics applications. With a period of early and exclusive access to new software developed in the Consortium, members enjoy a competitive advantage that can help them stand apart from their competition.

Pressure for a Plan

In the fourth edition of The Nanotech Report™, Lux Research reports that global government funding for nanotechnology research in 2005 was $4.61 billion, while corporate R&D investment reached $4.47 billon[1]. It's therefore no surprise that a survey of thirty-three multinational manufacturing, electronics, and life sciences corporations with revenues in excess of $5 billion (2003, median), found that 26% of corporations prioritized nanotechnology as one of their "top three" priorities, while 42% considered it a "high" priority[1]. It may be surprising, however, that only 45% of the companies surveyed felt they had an explicit strategy for applying nanotechnology within their organization[1].

With nanotechnology expected to spread exponentially within the manufactured goods market in the next ten years, and an estimated three to ten year gap between initial R&D and productization, companies with a strategy that enables them to move quickly and take advantage of a period of exclusivity stand to reap the most benefit from applying nanotechnology in products[1]. However, even with a clearly defined strategy for exploiting nanotechnology, companies face another challenge—nanotechnology research and development has largely lacked a rational design approach.



> **"We are excited about both the potential increase in the efficiency and effectiveness of our own R&D efforts, as well as the opportunity to fulfill the promise of enhanced rational design software tools."**
>
> David Morse
> VP of R&D at Corning and
> Accelrys Nanotech Consortium member

A Rational Approach to Nanodesign

Experimental research in nanotechnology tends to be very costly. Nanomaterials are very expensive and experimental characterization is often difficult because the behaviour and properties obtained from different synthesis and manufacturing methods can vary greatly. On top of this, structure-property relationships at the nanoscale are poorly understood. As such, *in silico* testing of material candidates, their assembly, and device properties has the potential to provide direction, as well as significant cost savings.

Maximizing Return on Investment

When integrated into a company's research and development efforts, software solutions have been shown to yield a significant return on investment. An IDC analysis of modeling software applied at chemical companies, including several Fortune 500 companies, found that:

Companies investing in modeling software in partnership with traditional experimentation realized a cumulative return on investment (ROI) on the order of $3 to $9 for every $1 invested in software tools and associated expenses[2].

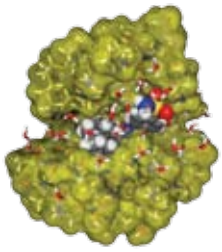
To cite a specific example, e2V technologies, a leading supplier of point-of-care and lab-on-a-chip products, has used Accelrys software to optimize the design of a biomarker detection system. Modeling allowed them to attain 100-fold optimization and accelerate the commercialization of their lab-on-a-chip product.

The Accelrys Nanotechnology Consortium

Recognizing the challenges facing organizations who are undertaking advanced materials and nanotechnology research, and the benefits a rational approach to nanodesign could bring, Accelrys, its scientific advisors and customers joined together to form the Accelrys Nanotechnology Consortium in July 2004.

The Consortium gives members the opportunity to work in collaboration with scientific thought-leaders to steer Accelrys' development of leading-edge modeling and simulation software technology. It aims to give members a competitive market advantage by providing exclusive rights to technology that enables them to:

- *Study systems at previously impossible levels of scale, accuracy, and complexity*
- *Quickly and efficiently set up calculations for such systems, minimizing costs typically seen with setting up such calculations*
- *Streamline and integrate complex analysis tasks through automated workflows*



Model of an inhibitor molecule bound to a complex of cyclin-dependent kinase CDK2. This complex including solvation water molecules contains 838 atoms. The binding energy was calculated to very high accuracy using ONETEP as part of a CDK inhibition study. For further details see Ref 5.

Phase I Progress Overview

The Consortium is an ongoing project, arranged into phases lasting approximately three years each. As illustrated in the table below, significant progress has already been made in Phase I, which is set to run through August 2007.

Ongoing Developments in Phase I

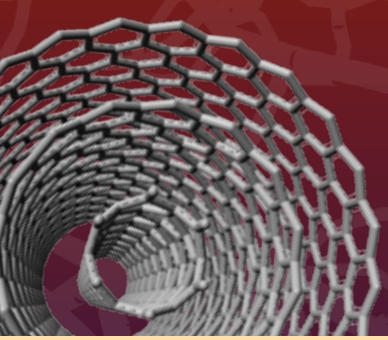
In addition to enhancing the functionality of existing deliverables, in particular ONETEP and GULP, further progress is underway to address member requirements for:

- *Hybrid simulations*
- *Forcefield coverage*
- *Workflow protocols in the area of surface science that streamline the determination of adsorption*

Nanotechnology Consortium Phase II

Accelrys, its advisors, and members are currently developing plans for a Phase II, which will run from 2007 to 2010. Phase II will continue to deliver leading-edge technologies for studying large-scale, complex systems and validated, streamlined protocols for complex tasks. Based on the technology foundations achieved during Phase I, Phase II will also focus more on technology integration, with goals to deliver flexible software solutions that address the advanced materials and nanotechnology-based industries' need for a more design-oriented approach to nanotechnology, in other words, delivering Computer Aided Nanodesign (CAN).

Phase I Goal	Consortium Deliverable	Application Examples
Construct complex nanostructures	New nanotube and nanocluster builders have been integrated into Materials Studio®, Accelrys' premier suite of modeling and simulation software for materials and chemicals research.	• Nanotubes as electromechanical sensors[3] • Nanoparticle catalysts
Access much larger systems (> 1000 atoms) with quantum accuracy	The new ONETEP linear scaling DFT method has been implemented for the members; this breakthrough technology allows high accuracy studies of systems much larger than has been possible with existing codes; this code, which is the result of over ten years of research and development at Cambridge University, has been secured exclusively for Consortium members.	• Calculation of properties of doped or functionalised nanotubes[4], nanoparticles • Study of reaction transition states in complex materials and biological systems • Determination of kinase inhibitor potencies[5]
Access a wider range of materials and properties, and include very large systems (>100,000 atoms) in classical simulations	A new version of GULP, a leading-edge classical simulation tool that complements DFT methods and enables a very wide range of property calculations on complex materials, has been delivered to members.	• Study of radiation damage in oxides[6] • Examination of the surface structure of semiconductors, sensors, and catalysts under environmental conditions[7]



Consortium Members and Advisors

The Consortium now has nine scientific advisors from Australia, Europe, Japan and the Unites States, and over twenty members from world-leading commercial companies, research organizations, and academic institutions. Over the first phase, resources from membership fees have allowed re-investment in Consortium software development, which is undertaken by an Accelrys research and development team that is dedicated to the Consortium.

"Whilst catalysis has always involved nanotechnology, the ability of atomistic modeling to impact this field is only relatively recent. Membership in the Accelrys Nanotechnology Consortium provides us with the ability to direct and influence how new state-of-the-art software products evolve. We are now able to access the products we need far quicker than would normally be anticipated."

Sam French
Senior Scientist at Johnson Matthey TC and
Accelrys Nanotech Consortium member

Why Join?

- *Ability to formally influence the direction of technology development and align these developments with your critical R&D needs*
- *Competitive advantage and an industry leadership position in applying new computational technology*
- *Early, exclusive, and unlimited access to new software developed by the Consortium (available to members prior to commercial availability)*
- *Perpetual rights to all Consortium deliverables (value of which exceeds membership fee)*
- *Access to exclusive meetings, training, and discussion workshops with world-leading scientific advisors and collaborators*

Making the Consortium Part of Your Strategy

Accelrys' twenty years of experience in providing rational design software for the chemicals and materials industries, along with its unique capabilities in application integration and its quality R&D and services departments, make it an ideal partner for your strategic approach to applying nanotechnology within your organization.

Current Consortium Advisors

Professor Richard Catlow
The Royal Institution, UK

Professor Mike Payne
University of Cambridge, UK

Professor Tim Clark
University of Erlangen, Germany

Professor Rubén Pérez
Autónoma University, Spain

Professor Julian Gale
Curtin University, Australia

Dr. Alessandro de Vita
Kings College London, UK

Professor Sharon Glotzer
University of Michigan, USA

Professor Alan Windle
University of Cambridge, UK

Professor Yoshiyuki Kawazoe
Tohoku University, Japan

For more information on the Accelrys Nanotechnology Consortium, including a full proposal, please contact **Dr. Gerhard Goldbeck-Wood, Consortium Director,** at **nanocon@accelrys.com.**

1. "The Nanotech Report™ 4th Edition," Lux Research, **2006**.
2. IDC Chemical Industry Market Study # 4158, **July 2004**.
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5. Heady, L., Fernandez-Serra, M., Mancera, R. L., Joyce, S., Venkitaraman, A. R., Artacho, E., Skylaris, C.-K., Ciacchi, L. C., Payne, M. C., "Novel structural features of CDK inhibition revealed by an ab initio computational method combined with dynamic simulations," *J. Med. Chem.*, **2006**, *49(17)*, 5141-5153.
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