

New software tools for Rational Nanomaterials Design: the Accelrys Nanotechnology Consortium.

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Nanomaterials by Design has been identified as a key strategic priority, both by industry and government. It is for example the topic of a major report of the US Chemical Industry Vision2020 Technology Partnership. The report provides a roadmap for taking technology from its current scientific discovery stage to an engineering discipline, in order to deliver on its economic promises. Modeling, Simulations and Informatics are identified as fundamental to the strategy and implementation of this vision.

The presentation will discuss the status and potential development of software tools to support such a strategy. It will discuss in particular the requirements to provide tools that increase accuracy of large size scale calculations, access complex time-dependent phenomena such as defect dynamics and handle non-equilibrium conditions. Potential solutions from leading academic groups will be outlined, including a new linear-scaling DFT method and a novel *Learn-on-the-fly* multiscale method. A software tool development strategy via the new Nanotechnology Consortium from Accelrys will be presented.

Further information is available at: <http://www.accelrys.com/consortia/nanotechnology/>

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