Workshop: Morphology and Crystal Structure Prediction using Materials Studio 4.4

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Wednesday September 2nd 2009, 14:00 – 17:00

Crystallisation processes are relevant to a wide range of industries such as chemicals, paints, explosives, food, and pharmaceuticals. The macroscopic properties of materials, such as the bioavailability of drugs, the taste of chocolate, or the colours of pigments and dyes, are all affected by the way their components crystallise. Scientific insight into crystal growth is also valuable in helping to control processes like scale inhibition and cement setting.

Accelrys provides simulation tools that help researchers to investigate and predict crystal structures and crystal growth and to design crystallization additives. Materials Studio's analytical and crystallization software helps you to investigate, predict, and modify crystal structure and crystal growth. You can simulate and explain particle morphology, predict crystal structure and understand polymorphism, study critical surface interactions, and design growth mediating additives.

In this workshop you will learn how to:

- Simulate and explain particle morphology. Accelrys' morphology prediction methods compute crystal shape based on the atomic-level structure by performing molecular mechanics-based energy calculations to determine the growth rates of different crystal faces.
- Predict crystal structure from powder diffraction patterns. Accelrys provides a complete package of modelling, powder diffraction simulation and refinement tools. Thousand of trial crystal structures can be generated and their simulated diffraction pattern compared to the experimental data, the structure generation being guided towards the best solution by global search algorithms. Best candidates can be refined to match the experimental data.

All Indaba6 attendees are welcome to participate to the Accelrys Workshop. Please bring your own laptop to participate to the hands-on session of Materials Studio 4.4. See system requirement here:
http://accelrys.com/products/materials-studio/system-requirements.html