Ab initio modeling for the design of TCO's: structural properties

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When properly done, the combination of experiments and ab initio modeling can speed up materials research. In this lecture, we outline the conceptual basis behind density functional theory and assess the accuracy and precision of this formalism, we discuss the prerequisites for a successful combination of modeling and experiment, and we illustrate this with a crystal structure prediction study that is relevant for the development of ZnO:Al.

Invited lecture for the following one-day workshop:

The future of transparent conducting oxides
Tuesday 26th August 2014, 10:00 – 16:30
Venue: Hasselt University – Martelarenlaan 42 – B-3500 Hasselt

A slidecast of this lecture is available at http://youtu.be/Wzu0TBVOFG4