

Ab initio in nanoelectronics industry

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Various trends in the electronics industry are systematically rendering the conventional macro and mesoscopic modeling methods less effective. The dimensions of typical modules are rapidly dropping into the nanometer range requiring the need for a full quantum treatment. Good old silicon is more and more replaced by new materials. For these, the fundamental knowledge is lagging too much to provide the parameters for compact modeling. The use of flexible substrates and increasingly complex modules in the back end of line puts strict limits on the processing temperatures. These are, in most cases, well below those that are required to anneal the involved materials into the crystalline phases. Fundamental knowledge of the resulting amorphous phases is however even less well developed.

Ab initio modelling can provide the needed intel to use a base for compact modeling and improve the needed fundamental understanding needed for real progress. The application of ab initio methods in this field however also pushes the current implementations to their limits.

In this presentation an overview and a series of examples is presented to make academic developers more aware of the needs from and the challenges faced in industry.