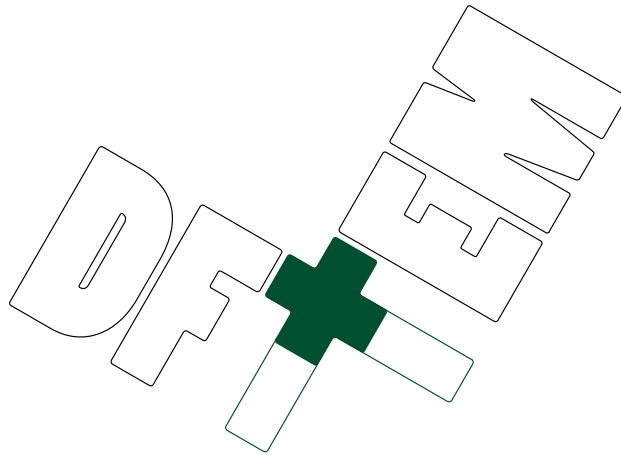


Joachim Luitz et al. (Eds.)

## **DFTEM 2006 – bringing together two communities**

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## Analysis and Design of Materials-Processes for Future Transistors

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The ongoing miniaturization of semiconductor devices requires the replacement of the conventional SiO<sub>2</sub>-based gate oxides by so-called high-k oxides, in order to avoid quantum mechanical leakage currents through an ultra-thin gate oxide. We discuss the route towards formation of epitaxial high-K oxides with silicon using state-of-the-art electronic structure calculations and ab-initio molecular dynamics simulations. I will describe the interesting interplay of metal atoms with the silicon dimers of the Si(001) surface, leading to sequence of phases as function of coverage. Then the interface structures between SrTiO<sub>3</sub> on silicon will be discussed. Special attention will be given on the interface chemistry and the requirements for obtaining an electronically inactive interface. We show that the band-offsets can be engineered for some of the interfaces by controlling the oxygen content at the interface. This is particularly important for the SrTiO<sub>3</sub>/Si(001) interface, which otherwise suffers from unacceptably low injection barriers.

New developments in semiconductor technology aim at introducing new semiconductors into silicon technology. This requires growth of high-mobility semiconductors such as Ge onto buffer oxides such as SrHfO<sub>3</sub>. Semiconductor growth on oxides suffers from clustering on the surface. We will show detailed studies of a potential process that shall allow epitaxial growth of Ge on SrHfO<sub>3</sub> using surfactants in molecular beam epitaxy.

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