Density Functional Theory of High-K Dielectric Gate Stacks.

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The semiconductor industry is responsible for much of the world's extraordinary economic expansion over the past fifty years. However, as the industry matures, the rate of innovation tends to saturate, and so does the growth. To continue scaling semiconductor devices below 45 nm, radically new materials need to be introduced into Si-dominated technology. One of the most active areas of research and development is a search for a new gate dielectric (so-called high-k dielectric) with a dielectric constant higher than that of silicon dioxide and silicon oxynitride. Transition metal (TM) oxides and in particular hafnium dioxide quickly emerged as leading candidates to replace SiO2. However, the intrinsic complexity of these materials has been underestimated, which made their integration into Si processing rather difficult. The rich physics and chemistry of TM oxides come from the presence of d-electrons. Being credited for the high polarizability and therefore a large dielectric constant (thus high-k) of the material they are also responsible for lattice instabilities, multiple charge state defects, and rather daunting interface chemistry. Another complication arises from the early decision to use a dual metal solution for the gate electrode.

Theoretical work and especially materials models based on density functional theory added much to our understanding of TM oxides and their interfaces with Si and other semiconducotrs, SiO2 and various metals in the context of semiconductor manufacturing. In this talk I will review recent progress in the ab-initio theory of high-k dielectrics, and outline the main ideas of the modern theory of polarizability, Schottky barriers, and correlated electrons as they are applied in materials research. In particular, I will describe studies of the dielectric response and its relation to the local stoichiometry, of oxygen related defects such as vacancies and of band discontinuities at various interfaces. I will focus on the analysis of the thermodynamics and electronic structure of hafnia interfaces with semiconductors, oxides and metals performed in my group.

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