First-principles study of Si CMOS materials and nanostructures

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***Abstract*—The technology roadmap reflects that complementary metal-oxide-semiconductor field-effect transistors based on silicon will reach absolute limits on its performance within the next decade. In microelectronics, quantum effects become important and the device performance is very sensitive to defects at or close to interfaces. To improve the device operation, it is urgent to understand materials, defects, and interface properties at the atomic level. First-principles calculations, based on the density functional theory, enable us to investigate important aspects of the physics of materials and structures. We will discuss successful applications and limitations of the modern computational techniques, such as the standard generalized gradient approximation, hybrid density functional, and quasiparticle energy calculations, for the electronic and transport properties and the role of defects in Si CMOS devices with Si/high-k and metal/high-k interfaces.**

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