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Electronic structure calculations for industrial technology development

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As computer technology advances, the role of modern electronic structure methods in industrial technology development becomes increasingly important. Such methods, based on density-functional theory (DFT), can provide deep insight towards understanding the challenges of the incorporation of novel materials for future technology nodes. DFT provides a framework in which bulk properties like band offsets, dielectric constant, and phonon spectra can be evaluated as well as properties associated with defects, such as fixed charge, migration barriers and mid-gap states. The computation of such properties is necessary for full evaluation of novel materials being reported by the industry as options to improve transistor performance.