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Theory of structural and dielectric properties of amorphous high-K dielectrics DAVID VANDERBILT, Rutgers University, DAVIDE CERESOLI, Rutgers University — Hafnia (HfO_2) and zirconia (ZrO_2) are leading candidates for replacing SiO_2 as the gate insulator in CMOS technology. Amorphous versions of these materials (a-HfO_2 and a-ZrO_2) can be grown as metastable phases on top of a silicon buffer; while they tend to recrystallize during subsequent annealing steps, they would otherwise be of considerable interest because of the promise they hold for improved uniformity and electrical passivity. In this work, we report our studies of a-HfO_2 and a-ZrO_2 by first-principles density-functional methods. We construct realistic amorphous models by two different techniques: (i) a "melt-and-quench" molecular dynamics approach, and (ii) an "activation-relaxation technique" (ART). In both cases, the structural, vibrational, and dielectric properties of the resulting models are analyzed in detail. The overall average dielectric constant is computed and found to be comparable to that of the monoclinic phase. Although the ART technique (as implemented by us in the SIESTA package) allows a dramatic saving in computational time, it yields results of similar quality with respect to ab-initio MD simulations done with the VASP code. These techniques show promise for future modeling of high-K dielectric ultrathin films and interfaces

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