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Anomalous behavior of the dielectric constant of hafnium silicates CARLO ANTONIO PIGNEDOLI, ALESSANDRO CURIONI, WANDA ANDREONI, IBM Research, Zurich Research Laboratory, 8803 Rueschlikon (Switzerland) — Hafnium silicates (HfSiO) are among the materials most frequently investigated in the search for a replacement of silicon dioxide as gate dielectric in CMOS devices. Measurements of the dielectric constant as a function of the relative concentration of the two binary oxides exhibit an anomalous behavior. Large-scale DFT-based calculations reveal that this is due to the change of the relative stability of different structures with composition and their strong influence on the permittivity. These results also help to rationalize the wide scatter in the experimental data for the dielectric constant for some concentrations and suggest ways to optimize the integration of these materials in the device.

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