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Point defect chemistry in amorphous HfO$_2$[1] R. RAMPRASAD, CHUNGUANG TANG, University of Connecticut — Neutral and charged native point defects in amorphous HfO$_2$ were studied using first principles computations. Thermodynamically, positively charged O vacancies and negatively charged Hf vacancies are the most probable point defects over a large atomic and electronic chemical potential range. Moreover, of all point defects, the positively charged O vacancy is the one with the lowest migration barrier. Hence, this point defect is identified as the most dangerous one in amorphous HfO$_2$ within the context of high-K gate dielectric applications in microelectronics.

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