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Doping in Si/SiO_2 Structures: A first-principles metadynamics study NICHOLAS LANZILLO, Rensselaer Polytechnic Institute, PHILIP SHEMELLA, IBM Research - Zurich, SAROJ NAYAK, Rensselaer Polytechnic Institute, WANDA ANDREONI, ALESSANDRO CURIONI, IBM Research - Zurich, RENSSELEAR POLYTECHNIC INSTITUTE COLLABORATION, IBM RESEARCH - ZURICH COLLABORATION — Dopant diffusion in semiconductor devices is a field of study with tremendous technological importance. We have performed first-principles metadynamics simulations of the diffusion of n-type dopants at the Si/SiO_2 interface using the ab-initio MD method. After the generation of a vacancy in the Si region, arsenic, phosphorus and silicon atoms show varying mechanisms of diffusion, including both substitutional and interstitial. Although at the near-interface silicon region arsenic is the first to diffuse interstitially, its interstitial position is more stable and thus less likely to diffuse across the interface relative to phosphorus and silicon. As arsenic crosses the interface, however, its relative stability decreases with respect to phosphorus and silicon and diffusion into the oxide becomes unfavorable. This is in agreement with experimentally observed arsenic pile-up at the Si/SiO_2 interface. We quantify the diffusion mechanisms by comparing free energy barriers in the silicon region as well as at the interface. We find the largest barriers exist for silicon, while the smallest barriers exist for arsenic.

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