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**Ab-Initio Study of the Effect of Hydrogen and Point Defects on Arsenic Segregation at Si (100)/SiO2 Interfaces** KARTHIK RAVICHANDRAN, WOLFGANG WINDL, TAO LIANG, Department of Materials Science and Engineering, The Ohio State University, 2041 College Rd., Columbus, OH, 43210 — The previously suggested segregation model for arsenic at $Si/SiO_2$ interfaces based on a combined trapping/pairing model [J. Dabrowski *et al.*, Phys. Rev. B **65**, 245305 (2002)] requires high binding energies for interface vacancies, which our results of $\approx$ 0.2 eV cannot confirm. As an alternative explanation, we present ab-initio results which show that As and hydrogen bond with an energy gain of 1.5-3 eV with their minimum-energy position at the interface, which creates additional trapping sites for As segregation. We also find a similar situation in case of boron segregation. The inclusion of hydrogen into the modeling might thus be able to explain the differences between the previous model and experiments.

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