

ARTICLE

Supplementary Information

Gamma-ray Irradiation Induced Oxidation and Disproportionation at the amorphous SiO₂/Si Interfaces

Dechao Meng,^{*,†,ab} Mu Lan,^{†,ab} Zeng-hui Yang,^{ab} Shouliang Hu,^b Guanghui Zhang,^{ab} Chuanhui Liang,^c Haoran Zhan,^d Jiang Liu,^d Ming Li,^b Hang Zhou,^{ab} Xu Zuo,^e Yu Song^{ab} and Su-Huai Wei^{*,†}

^aMicrosystem and Terahertz Research Center, China Academy of Engineering Physics, Chengdu 610200, China E-mail: mengdechao@mtrc.ac.cn

^bInstitute of Electronic Engineering, China Academy of Engineering Physics, Mianyang 621999, China

^cInstitute of Materials, China Academy of Engineering Physics, Chengdu, Sichuan, 610200, China

^dChengdu Green Energy and Green Manufacturing Technology R&D Center, Chengdu Development Center of Science and Technology, Chengdu 610200, China.

^eCollege of Electronic Information and Optical Engineering, Nankai University, Tianjin 300071, China

^fBeijing Computational Science Research Center, Beijing 100094, P. R. China E-mail: suhuaiwei@csrc.ac.cn

† The authors contribute equally to this paper.

* Corresponding authors.

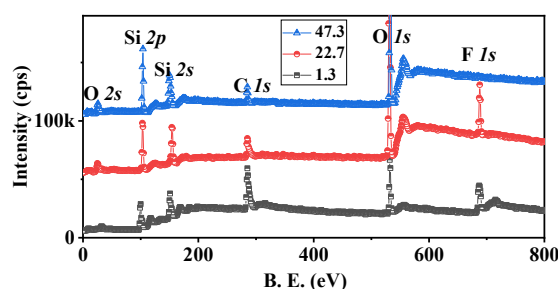


Figure S1. XPS survey results of three typical films with all the elements marked.

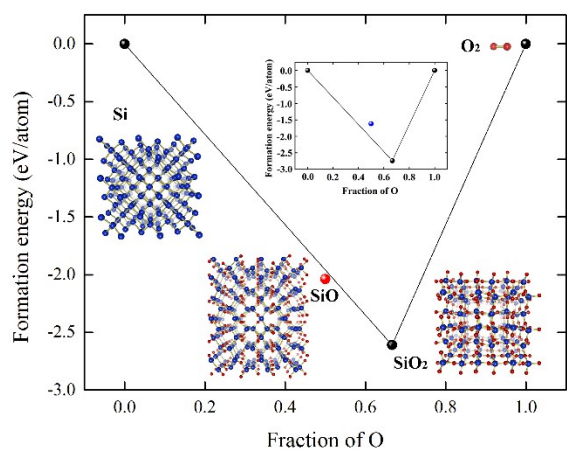


Figure S2. The phase diagram of Si-O calculated with ReaxFF. The formation energy of SiO is below the Si-SiO₂ line, which means the ReaxFF erroneously finds SiO being thermally stable and disallowing disproportionation energetically. For comparison, top inset depicts phase diagram calculated using DFT with the HSE functional. The formation energy of SiO is above the Si-SiO₂ line, showing that SiO is unstable and can decompose into SiO₂ and Si phases.