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Structural properties and electronic structures of amorphous HfO_2/Si(001) interface CHEN GUOHONG, HOU ZHUFENG, GONG XINGAO, Surface Physics Laboratory and Department of Physics, Shanghai-200433, XG-GONG'S GROUP TEAM — Using the projector augmented wave method within the generalized gradient approximation, we have performed *ab-initio* molecular dynamics simulations to generate an atomic structure model of amorphous hafnium dioxide (a-HfO_2) by a melt-and-quench scheme, and have investigated the structural and electronic properties of a-HfO_2 /Si(001)-$c(2\times2)$ interface. The structure of a-HfO_2 sample is analyzed via atomic coordination number and partial pair-radius distribution functions. Our results show the average Hf-O nearest-neighbor distance is 2.06 ?, which is comparable with the Hf-O bond lengths (in the range from 2.04? $\sim$ to 2.25?) in monoclinic HfO_2 crystalline, and also indicate the generated sample essentially reflects the experimentally measured structural characteristics of a-HfO_2. Most importantly, it is found that the valence band offset of a-HfO_2/Si interface is about 2.97eV, and our results suggest that the coordination of Si atoms at interface would significantly affect the electronic properties of interface.

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