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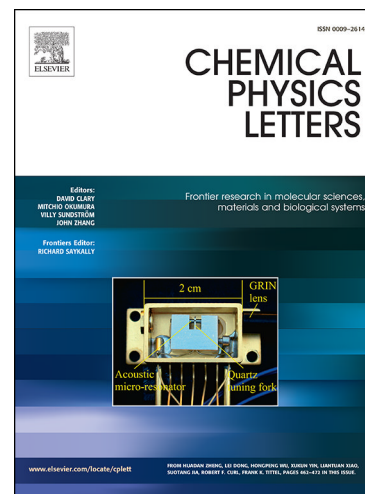
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Hydrogen-/fluorine-passivation effects in amorphous silica fiber

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Abstract: We present first-principles combined GW and Bethe-Salpeter equation on passivation effect between ODC(I) and H/F atoms. The injection of H or F atoms help to form the robust Si-H or Si-F bond which increase the optical band gap, erase the defect state of ODC(I) at 0.74 eV and improve radiation toughness. The reaction of ODC(I) defect with a H atom or F atoms is barrierless, the Si-O length near the ODC(I) sites are all gradually getting shorter and bond energy are getting stronger. Coupled with the atomic structures and electro-optic properties, we found out that F is the better passivator.

Keywords: first principles, silica fiber, ODC defect, passivation

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