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Direct Detection of Interstitial Oxygen and its Electronic Structure in Superconducting $Fe_{1+y}TeO_x$ Thin-Films JIAN-MIN ZUO, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, HEFEI HU, Condensed Matter Physics and Material Science, Brookhaven National Laboratory, MAO ZHENG, CAN ZHANG, LAURA GREENE, JAMES ECKSTEIN, Department of Physics, University of Illinois at Urbana-Champaign, JI-HWAN KWON, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — $Fe_{1+y}Te$ thin films become a superconductor when doped with oxygen, in which the interstitially incorporated oxygen plays crucial role for emergence of superconductivity. In this study, we investigated atomic and electronic structure of the oxygen-doped $Fe_{1+y}Te$ thin films using electron energy loss spectroscopy (EELS) and first principles calculation based on density functional theory (DFT). Atomic-resolution EELS reveals interstitial oxygen position next to the Fe layer, four fold hollow site, which location is consistent with DFT calculation result showing that the experimentally-found structure is the most energetically stable interstitial site. The relaxed geometry of oxygen-incorporated FeTe through DFT calculation shows drastic structural distortions in the planar structure of FeTe layer, which is associated with large amount of magnetic moment fluctuation in the Fe atoms with the bicollinear antiferromagnetic configuration. The detailed analysis including the charge density and electronic structures of the oxygen-doped FeTe will be presented.

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