Pressure Dependence of Electron Structures and Spin States in $Fe_{1.01}Se$ Superconductors Probed by X-ray Absorption and X-ray Emission Spectroscopy

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Pressure dependence of electron structures and spin states of iron-chalcogenide $Fe_{1.01}Se$ superconductors up to ∼66 GPa has been investigated with x-ray emission spectra and x-ray absorption spectra with partial-fluorescence yield. The intensity of the pre-edge peak at ∼7112.7 eV of the Fe K-edge x-ray absorption spectrum of $Fe_{1.01}Se$ decreases progressively with pressure up to ∼10 GPa. A new pre-peak at energy ∼7113.7 eV develops for pressure above ∼13 GPa, indicating formation of a new phase. The larger compression accompanied with a significant distortion around the Fe atoms along the c axis in $Fe_{1.01}Se$ upon applying pressure suppresses the Fe $3d$-Se $4p$ and Fe $4p$-Se $4d$ hybridization. The applied pressure suppresses the nearest-neighbor ferromagnetic superexchange interaction and enhances spin fluctuations on the Fe sites in $Fe_{1.01}Se$. A discontinuous variation of the integrated absolute difference (IAD) values of the $K\beta$ emission line was observed, originating from a phase transition of $Fe_{1.01}Se$ for a pressure above 12 GPa. $Fe_{1.01}Se$ shows a small net magnetic moment of Fe^{2+} at ambient pressure, probably arising from strong Fe-Fe spin fluctuations. The satellite line $K\beta'$ was reduced in intensity upon applying pressure and became absent for pressure >52 GPa, indicating a loss of magnetic moment of $Fe_{1.01}Se$ superconductors.