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Valence Band Character of $NiS_{2-x}Se_x$ using 3p-3d Resonant ARPES GARAM HAN, YEONGKWAN KIM, YOONYOUNG KOH, BEOMYOUNG KIM, DONGJOON SONG, JUNGJIN SEO, WONSHIK KYUNG, Institute of Physics and Applied physics, Yonsei university, Korea, KYUNGDONG LEE, Department of Physics, Inha university, Korea, CHANGYOUNG KIM, Institute of Physics and Applied physics, Yonsei university, Korea — Understanding the strong correlated system is one of the most challenging tasks in condensed matter physics. Especially, the metal insulator transition (MIT) has been one of the major topics recent few decades. $NiS_{2-x}Se_x$ is known as one of famous material which has MIT. The cubic pyrite NiS_2 is a charge-transfer (CT) insulator. NiS_2 attracts particular interest as it easily forms a solid solution with $NiSe_2$ ($NiS_{2-x}Se_x$) which, while being isoelectronic and isostructural to NiS_2, is nevertheless a good metal. MIT, induced by Se alloying, is observed at low temperature (T) for x=0.45. Perucchi and his collaborators revealed closed relation between MIT and band width through comparison of infrared spectroscopy result and LDA calculation. However, it was only an indirect observation, and is inconsistent with recent proposal that NiS_2 is not a CT insulator but an insulator due to the bonding-antibonding splitting in the S – S (Se – Se) dimers. To reveal the true mechanism in the MIT in $NiS_{2-x}Se_x$, resonant photoemission experiment is essential. According to competing theories (CT insulator and insulator due to bonding-antibonding splitting), it is expected that the character of the main band that is responsible for the MIT should be different. Therefore, we performed 3p->3d resonant ARPES for various Se dopings (x=0.43; insulator, x=0.5, 0.7, 2.0; metal) and observed a significant change between on- and off-resonances near the MIT. Our experimental result supports that the origin of MIT in $NiS_{2-x}Se_x$ is the CT theory rather than the dimer theory.

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