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Study on the correlation between s± pairing and intra-orbital spin fluctuations in 1111 iron based superconductors with isovalent doping HIDETOMO USUI, KATSUHIRO SUZUKI, KAZUHIKO KUROKI, Department of Physics, Osaka University — Recently, 1111 iron based superconductors with isovalent doping have been experimentally investigated in $LnFeAs_xP_{1-x}O_{1-y}F_y$ (Ln=La, Nd, Pr) [1-4]. Interestingly, it was found that T_c takes its local maximum in the intermediate regime of arsenic/phosphorous ratio, which indicates that the superconductivity is locally optimized at a certain Fe-Pn-Fe (Pn=Pnictogen) bond angle larger than 109 deg. Given this background, we study the correlation between the local lattice structure, the orbital character of the Fermi surface, and T_c in 1111 system with isovalent doping. We calculate the band structure of $LnFeAs_xP_{1-x}O_{1-y}F_y$ and construct effective five orbital models. To our surprise, it is found that superconductivity is indeed locally optimized in the intermediate arsenic doping regime. The origin of this local optimization is traced back to the gradual variation of the orbital character and the density of states of the hole Fermi surfaces around the Γ point, which is controlled by the bond angle. The consistency with the experiment strongly indicates the importance of the spin fluctuation played in this series of superconductors.

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