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Electronic structures of 122- and 111-type silicides and germanides in comparison to iron pnictide superconductors[1] YUKARI KATSURA, HIDENORI TAKAGI, Magnetic Materials Laboratory, RIKEN — Despite the high transition temperatures, iron pnictide superconductors have difficulty in practical use, due to high toxicity of pnictogens. Besides, the parent crystal structures of iron-based superconductors have been observed over wide range of constituent elements. In this study, we investigated the electronic structures of $ThCr_2Si_2$ (122)-type and CeFeSi (111)-type compounds containing Si or Ge instead of pnictogens. While superconducting $A Fe_2As_2$ (A: group 1-2 elements) has cylindrical Fermi surfaces with strong interband nesting, Fermi surfaces of isoelectronic compounds such as 'ACo_2Ge_2' did not have these characteristics, mainly due to distortion of the '$CoGe_4$' tetrahedra. We investigated the relationship between the crystal geometry and the chemical species of 122- and 111-type compounds, and calculated their effects onto the electronic structures. We found that 111-type phases tend to have smaller distortion of tetrahedra than 122-type phases, although more electron-deficient metals must be chosen in order to reproduce the electronic structures of the superconducting phases. We will suggest some compositions that are expected to reproduce such electronic structures, and report about the synthesis of these compounds.

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