Application of first principles methods in iron-selenide superconductors

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The discovery of vacancy-ordered iron-selenides has stimulated many interests in superconducting community. In this talk, we will present our electronic structure calculation results of these compounds, including 122 phase, 234 phase, 245 phase and 278 phase. The striking effect of ordered iron-vacancies and their relevance with respect to superconductivity will be discussed.