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Phase diagram of β' -BEDT-TTF salts HIORI KINO, NIMS, Japan, HIROSHI KONTANI, Nagoya Univ., Japan, TSUYOSHI MIYAZAKI, NIMS, Japan — We present theoretical studies on the phase diagram of layered organic charge transfer salts, β' -(BEDT-TTF)₂ICl₂ and β' -(BEDT-TTF)₂AuCl₂. The former shows the highest superconducting transition temperature (T_c 14.2 K under a high hydrostatic pressure) among the organic superconductors. We study an effective model using the fluctuation-exchange (FLEX) approximation based on the results of the first-principles calculations in DFT/GGA under applied pressures. In the obtained phase diagram of β' -(BEDT-TTF)₂ICl₂, the superconductivity with d_{xy} -like symmetry is realized next to the antiferromagnetic phase. The calculated T_c quantitatively coincides well with the experimental one.

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