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Multipolar effects in Eu2Ir2O7 YILIN WANG, XI DAI, Institute of Physics, Chinese Academy of Sci (CAS) — We use the density functional theory plus the rotationally invariant Hartree-Fock mean-field method to study the magnetic properties of the pyrochlore iridate material $Eu_2Ir_2O_7$ ($5d^5$), where the crystal field splitting Δ, spin-orbit coupling (SOC) λ and Coulomb interaction U of Ir atoms are all playing significant roles. We have constructed a t_{2g} Wannier tight-binding Hamiltonian and calculated the U-λ phase diagram, from which we find a very stable all-in/all-out antiferromagnetic ground state for moderate SOC (0.2-0.5 eV). In this magnetic state, except for the dipole moments, we also find considerable multipolar moments (octupole) and large non-linear magnetic susceptibility. With strong enough SOC, the system reduces to a $j_{eff} = \frac{1}{2}$ single band Hubbard model, and the ground state changes to another antiferromagnetic configuration without multipolar moments. Our results indicate that the coexisting multipolar order is crucial to stabilize the all-in/all-out state and contributes a lot to the non-linear magnetic susceptibility.

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