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Microscopic theory of multipole ordering in NpO_2 KATSUNORI KUBO, Advanced Science Research Center, Japan Atomic Energy Research Institute, TAKASHI HOTTA, Advanced Science Research Center, Japan Atomic Energy Research Institute — It has been a longstanding problem in physics of actinide compounds to determine the order parameter of the low-temperature ordered phase of NpO_2. Recently, several experimental facts have been found to be reconciled by assuming octupole ordering. To understand the origin of the octupole ordering, we construct an f-electron model on an fcc lattice based on a j-j coupling scheme, and derive an effective multipole-interaction model. By analyzing the effective model numerically, we determine the interactions relevant to the ground state. Then, we apply mean field theory to the simplified model including only these interactions, and find that the longitudinal triple-q Γ_{5u} octupole order is realized in our model by the combined effects of multipole interactions and anisotropy of the Γ_{5u} moment. We will discuss a possible relation between the present results and experimental observations for NpO_2.

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