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Strong Dzyaloshinskii-Moriya Interaction and Origin of Ferroelectricity in Cu₂OSeO₃¹ JI-HUI YANG, ZHENG-LU LI, XUEZENG LU, X.G. GONG, HONGJUN XIANG, Key Laboratory of Computational Physical Sciences (MOE), State Key Laboratory of Surface Physics, and Dept of Physics, Fudan University, Shanghai, M.-H. WHANGBO, Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204, USA, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — In this work, we try to understand the skyrmions recently observed experimentally in Cu2OSeO3 system, as well as its origin of ferroelectricity. Based on the spin Hamiltonian, we developed four-state-energy-mapping method to derive these spin interaction parameters. For this system, we found a very large ratio between the DM term and the symmetric exchange interaction. Besides, the spin arrangements in the ground state are found degenerate and the spin energy is independent of the propagation vector q. Taking these two factors into account, we explained the experimental observation of skyrmions to some extent. Then we built a model to describe the polarization of this system. By the symmetry analysis, the ferroelectricity is supposed to result from the spin single-site term, as is confirmed by direct calculations of our model. Using this model, we analyzed its ferroelectricity dependence of the spin arrangement and find the largest polarization happens when the spins are along <111> direction, in excellent agreement with the experimental results.

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