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Orbital order fluctuations in KCuF3

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Abstract

The interaction of orbital momenta of copper in KCuF3 via the field of elastic deformations is analyzed taking into account the local rotations of electron density on copper ions. It is found that the interaction energy related to local rotations of copper ions is comparable in order of magnitude with the Dzyaloshinskii-Moriya interaction energy. The calculated interaction energy of copper orbitals in the ab plane of the crystal exceeds the energy of their interaction along the c axis. This circumstance explains recently found specific features of orbital melting in LaMnO3 with increasing temperature. © 2014 Pleiades Publishing, Ltd.

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