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Realistic simulation of Kondo lattice model: application to Cerium compounds MUNEHISA MATSUMOTO, MYUNG JOON HAN, UC Davis, JUNYA OTSUKI, Tohoku University, Japan, SERGEY SAVRASOV, UC Davis — In order to do a good description of heavy fermion materials at very low temperatures, we simulate the Kondo lattice model with the continuous-time quantum Monte Carlo method recently developed by one of the authors [1] combined with the conduction-electron density of states given by first-principle calculations and performing self consistency using dynamical mean field theory. We discuss our results for Cerium compounds down to the temperature range of O(1) [K] using realistic values of crystal-field and spin-orbit level splitting. [1] J. Otsuki, H. Kusunose, P. Werner, Y. Kuramoto, J. Phys. Soc. Jpn. 76, 114707 (2007).

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