

Abstract Submitted
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Pressure-driven 4 f localized-itinerant crossover in heavy-fermion compound CeIn₃: A first-principles many-body perspective¹ HAIYAN LU, LI HUANG, Institute of Materials, INSTITUTE OF PHYSICS CHINESE ACADEMY OF SCIENCES COLLABORATION — The localized-itinerant nature of Ce-4*f* valence electrons in heavy fermion compound CeIn₃ under pressure is studied thoroughly by means of the combination of density functional theory and single-site dynamical mean-field theory. The detailed evolutions of electronic structures of CeIn₃, including total and partial density of states, momentum-resolved spectral functions, and valence state histograms are calculated in a wide pressure range where the corresponding $V/V_0 \in [0.6, 1.0]$ (here V_0 is the experimental crystal volume) at $T \cong 116$ K. Upon increasing pressure, two strong peaks associated with the Ce-4*f* states emerge near the Fermi level, and the *c-f* hybridization and valence state fluctuation are enhanced remarkably. Moreover, the kinetic and potential energies rise, while the occupancy, total angular momentum, and low-energy scattering rate of the Ce-4*f* electrons decline with respect to pressure. All the physical observables considered here exhibit prominent kinks or fluctuations in $V/V_0 \in [0.80, 0.90]$, which are probably the desired fingerprints for the Ce-4*f* localized-itinerant crossover.

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