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Modeling the Localized to Itinerant Electronic Transition in the Heavy Fermion System CeIrIn5

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Within the ab-inition calculation we adress the crossover from localized to itinerant state of a heavy fermion material CeIrIn5. The temperature evolution of the one electron spectra and the optical conductivity is predicted from first principles. The buildup of coherence in the form of a dispersive many body feature is followed in detail and its effects on the conduction electrons of the material is revealed. We find multiple hybridization gaps and link them to the crystal structure of the material. Our theoretical approach explains the multiple peak structures observed in optical experiments and the sensitivity of CeIrIn5 to substitutions of the transition metal element and may provide a microscopic basis for the more phenomenological descriptions currently used to interpret experiments in heavy fermion systems.