By employing a combined approach of the unity bond index–quadratic exponential potential method and density functional theory within the generalized gradient approximation, we have studied the interaction of intermediates in the ethanol dehydrogenation process to ethyl acetate on Cu, Ag, Ni, Pd, Pt, Co, Au and Ir(111) transition metal surfaces. Binding energies and geometries were optimized for the main intermediates of this process. Electronic structures were computed for some intermediates/transition metal systems. We also calculated the activation energies for the elementary steps of the reactions. The results show that amid the studied surfaces, Cu(111) stabilizes ethoxy and acetyl species, preventing their dissociation. Inducing the h_2 binding mode of acetaldehyde by alloying Cu with Ni, Co, Pd, Pt or Ir can enhance the catalytic proprieties of the Cu(111) clean surface.