Abstract:
The chemistry of ethylene on group VIII metals is important for the petrochemical and polymer industries. Thus far, a complete first-principles-based conversion network of ethylene as a prototypical olefin system on metal surfaces is lacking. In this paper we present a comprehensive view on transformations of ethylene on Pd(111), based on density functional slab model calculations. Specifically, we characterized the thermodynamics and kinetics of C-H and C-C bond scission as well as II isomerization of a series of species C(2)H(a) (}