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Direct versus hydrogen assisted CO dissociation on metal surfaces DOMINIC ALFONSO, National Energy Technology Laboratory - Department of Energy — We present investigations of the formation of precursor hydrocarbon species relevant to production of liquid hydrocarbons on low index surfaces of various important noble and transition metals. The formation could occur via the so-called carbide mechanism where direct CO dissociation takes place, followed by stepwise hydrogenation of C yielding CH_x species. Formation of precursor CH_x species could also potentially take place through hydrogenated CO intermediates. First-principles calculations of energetics and barriers of CO conversion to hydrocarbons species were performed using plane-wave periodic density functional theory. Our calculations indicate that the two pathways are generally competitive on transition metals. A microkinetic model, with input thermodynamics and kinetic parameters estimated from electronic structure calculations, has been developed. The two pathways will be further examined using microkinetic approach to determine whether the aforementioned finding holds at realistic conditions.

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