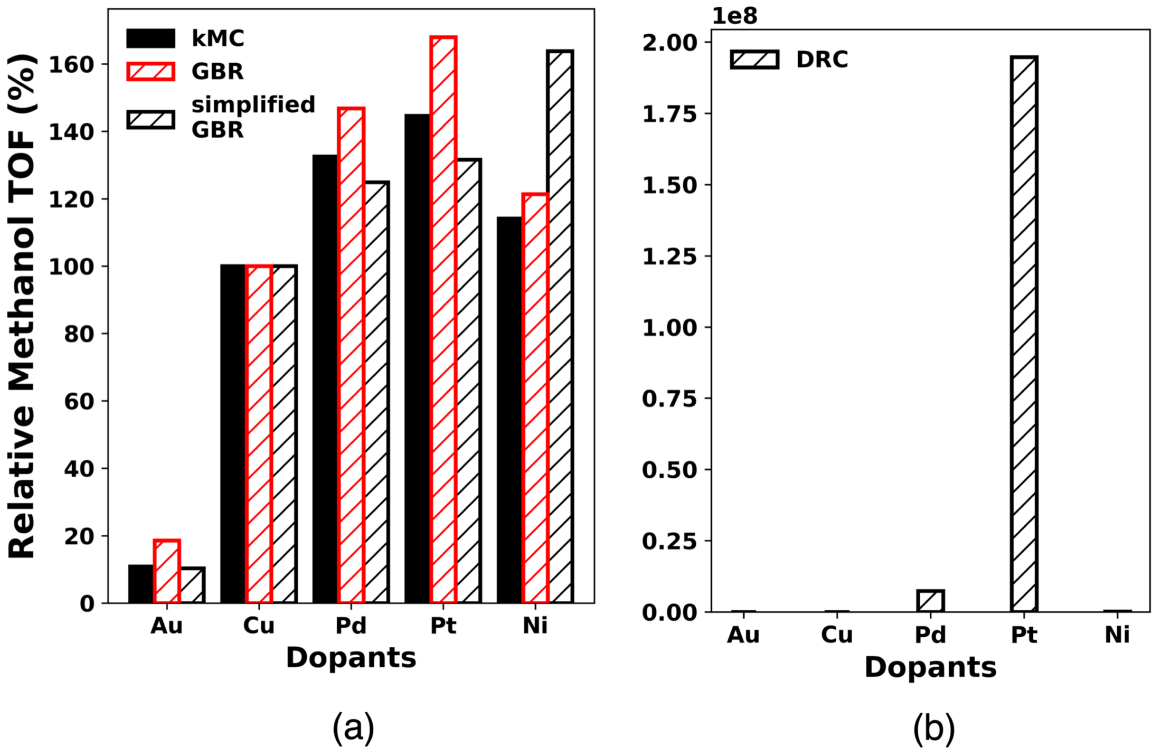

(a) (b)

Figure 1. (a) Comparison of the predicted methanol TOF from CO hydrogenation on M-doped Cu(111) between GBR model with both first-order and second-order descriptors (shadowed red bar) and simplified GBR model with first-order descriptors only (shadowed black bar) with the kMC simulated values (solid black bar) as criteria.(b) Predicted methanol TOF from CO hydrogenation on M-Cu(111) by DRC method. All TOFs are calibrated to the Cu(111) surface respectively.