M/TiC as a single atom elecrocatalyst for HER and ORR reactions: A DFT approach

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Significant progresses have already been made in the studies of single-atom catalysts and its use in electrocatalytic reactions have been actively studied because they can provide energy or chemicals in a more environmentally friendly way. In this regard, with the help of density functional theory (DFT) calculations, we explored the stability and activity of transition metal single atom on the TiC surface. We found the carbon vacancy, which is very common in experimental findings helps to stabilize these single atoms on the surface. Hydrogen evolution reaction (HER) activity of these catalysts have also been studied. We found that the activity of Ni as a single atom is very close to the conventional Pt catalyst. Meanwhile, the single atom catalyst can be used for H_2O_2 production through an environment friendly way. We also tested our model catalyst for this reaction. We found that Au and Pd have higher limiting potential than Pt for H_2O_2 production.