Contribution ID: **180** Type: **Talk**

【215】Polarons in Single Atom Catalysts: Case Study of Me1= [Au1 ,Pt1 ,Rh1] on TiO2(110)

Tuesday, 31 August 2021 17:30 (15 minutes)

Identification of the local environment of a single-atom catalyst on metal oxide surfaces is crucial for understanding the reactivity and the catalytic properties. On TiO_2(110), the stability and reactivity of adsorbed adatoms is further complicated by the presence of oxygen vacancies and associated polaron charge, as both can affect the electronic structure and local geometry. In this work the adsorption of atoms are studied by density functional theory (DFT+U) and compared with our experimental results (Rh_1) and with available literatures (Au_1 and Pt_1). By investigating the most stable adsorption site, oxidation state, O vacancies and polarons our data shows that Pt and Au fill oxygen vacancies, contrary to Rh.

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Session Classification: Surfaces, Interfaces and Thin Films

Track Classification: Surfaces, Interfaces and Thin Films