

The fight for a reactive site

Irene Groot, Leiden Institute of Chemistry / FOM Institute for Plasma Physics Rijnhuizen

Hydrogen dissociation on metal surfaces is an elementary step in many industrial heterogeneously catalyzed reactions. Here I will discuss the dissociation of hydrogen on Ru(0001), CO/Ru(0001), and stepped platinum surfaces.

Using supersonic molecular beam techniques the reaction probability of H₂ and D₂ on bare and CO-precovered Ru(0001) is measured as a function of kinetic energy, surface temperature and angle of incidence. The results for bare Ru(0001) are compared to 6D quantum dynamics results.

The reaction dynamics of H₂ dissociation on CO-precovered Ru(0001) is studied in detail applying DFT and quantum and quasi-classical dynamics calculations.

The dissociation of H₂ on stepped platinum is studied employing molecular beam techniques. Results for Pt(211) are compared to calculations for the same system. I present an overview of the different reaction mechanisms observed for H₂ dissociation, and using the assumption of step and terrace separation, I will show that the reactivity of Pt(533) and Pt(755) can be predicted from the measured reaction probability on Pt(211).