Investigating the deNO$_x$ ability of a stepped Rh {443} surface

Abstract:

The emission of nitrogen oxides (NO$_x$, $x = 1,2$) from combustion engines can damage the environment by forming acid rain in the atmosphere and contribute to the formation of smog at ground level. Efforts to combat these harmful emissions have led to the development of technologies to decompose NO$_x$ (deNO$_x$) to the more environmentally friendly N$_2$ and O$_2$ gases. These include the three-way catalytic converter for automobiles and a range of technologies for stationary diesel engines, such as selective catalytic reduction and NO$_x$ storage-reduction catalysts. Rhodium metal is typically utilised in these technologies as the reduction catalyst; however, its ore has become severely depleted and scarce, making it expensive. The {111} surface is the most stable of the low index surfaces and thus widely exposed for catalytic purposes. In reality, however, the Rh {111} surface is not entirely flat and possesses structural defects such as steps and kinks which can influence the rate of deNO$_x$. This study will use density functional theory calculations to investigate the ability of a stepped Rh {443} surface to break down NO$_x$ gases.