Topography and localized charge of steps on CeO_2(111) investigated by AFM/KPFM

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The configuration of step edges on metal oxide surface is significant for understanding fundamental reactivity and predicting the performance in catalysis. In this work, the topography feature and charge of steps on CeO_2(111) are investigated by atomic force microscopy /kelvin probe force microscopy combined with density functional theory. Hexagonal islands and pits containing step I edge and step II edge have been observed at annealing 1100 K. The irregular structures with the addition of step III edge have been found at 1200 K. The measurement of contact potential difference reveals that step II displays the strongest localized charge state, followed by step III, and step I with the weakest localized charge state. The calculations of density functional theory have confirmed that step II possesses a stronger localized charge state. In addition, the Ce atoms at the step II edge exhibit greater positive and negative charge accumulation. These results provide the surface structure and electrical potential of three step edges on the CeO_2(111), and establish both experimental and theoretical foundations for subsequent investigations on adsorption and catalysis.

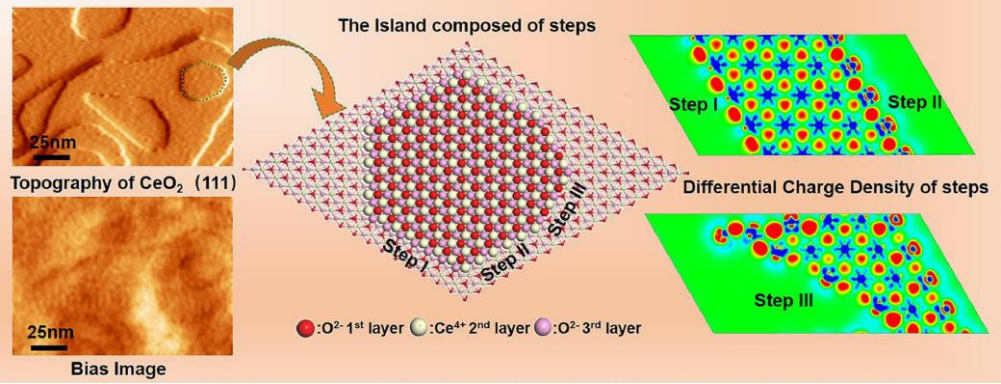

Figure 1. Topography and bias image of CeO_2 (111) surface by NC-AFM/KPFM at 1200 K. The scale mode corresponding to the island of CeO_2 (111) surface and deformation charge density of step I, II and III.

Reference

[1] Pengli. Shu, et al. Surfaces and Interfaces, 51, 104738(2024).