Favorable Pathway of O_2 Dissociative Adsorption on a Single Platinum Adatom Coated on Gamma-Alumina (111) Surface: A Density Functional Theory Study

Publons ID	37933893
Wos ID	WOS:000296085700057
Doi	10.1143/JJAP.50.105602
Title	Favorable Pathway of O_2 Dissociative Adsorption on a Single Platinum Adatom Coated on Gamma-Alumina (111) Surface: A Density Functional Theory Study
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Publish Date	OCT 2011
Journal Name	JAPANESE JOURNAL OF APPLIED PHYSICS
Citation	2
Abstract	We have investigated the dissociative adsorption process of O-2 (oxygen molecule) on a composite surface formed by coating a single platinum (Pt) adatom on a gamma-alumina (gamma-Al2O3) (111) surface. This process is studied by using density functional theory (DFT) and described in terms of potential energy surfaces (PES) with respect to the molecular degrees of freedom. We compare the activation barriers and adsorption energies among typical reaction channels. Our results show that O-2 dissociative adsorption is preferably occurred when this O-2 molecule approaches the surface with molecular orientation inclined by 30 degrees angle with respect to the surface normal, i.e., the condition with lowest activation barrier. The results indicate that dissociated O atoms are likely to form strong bonds with the Pt adatom by keeping distance from the alumina layer. (C) 2011 The Japan Society of Applied Physics
Publish Type	Journal
Publish Year	2011
Page Begin	(not set)
Page End	(not set)
Issn	0021-4922
Eissn	
Url	https://www.webofscience.com/wos/woscc/full-record/WOS:000296085700057
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