

## Accepted Manuscript

Title: Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principle

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PII: S0169-4332(16)32127-4  
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2016.10.032>  
Reference: APSUSC 34126

To appear in: *APSUSC*

Received date: 4-8-2016  
Revised date: 24-9-2016  
Accepted date: 5-10-2016

Please cite this article as: Bo Gao, Jianyun Wang, Jian Lv, Xingyu Gao, Yafan Zhao, Yanchao Wang, Haifeng Song, Yanming Ma, Novel structures of oxygen adsorbed on a Zr(0001) surface predicted from first principle, Applied Surface Science <http://dx.doi.org/10.1016/j.apsusc.2016.10.032>

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- Two stable structures of O adsorbed on a Zr(0001) surface are predicted with SLAM.
- A stable structure of O adsorbed on a Zr(0001) surface is proposed with MLAM.
- The calculated work function change is agreement with experimental value.

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