

Supporting Information

First-principles insights into atomic oxygen protection coatings composed of scale-like layered double hydroxide nanosheets

Denghang Tang ^{a, b}, Rui Sun ^{a, b}, Jiayu Zheng ^{a, b}, Mengyun Xu ^a, Haogeng Li ^a, Hongyu Gu ^{a, b, c, *},

Yuzhi Zhang ^{a, b, *}, Yi-Yang Sun ^{b, c}, Lixin Song ^{a, b}

^a *Research Center of Inorganic Coating Materials, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 201899, P.R. China;*

^b *Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, P.R. China;*

^c *State Key Laboratory of High Performance Ceramics, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 201899, PR China.*

*Corresponding Authors

E-mail: guhongyu@mail.sic.ac.cn (Hongyu Gu)

yzzhang@mail.sic.ac.cn (Yuzhi Zhang)

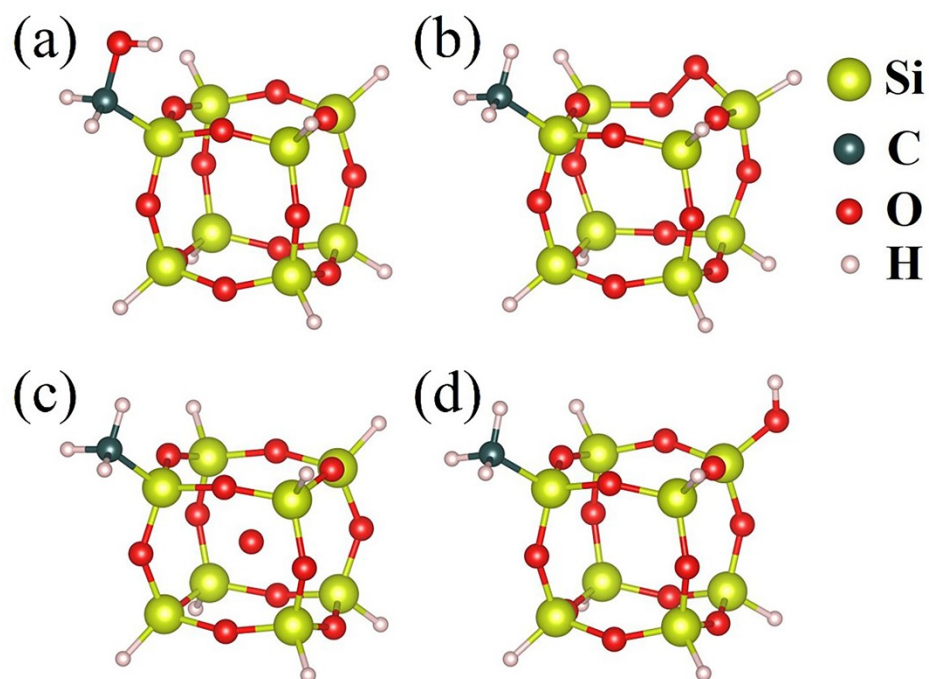


Fig. S1 The adsorption of AO on polysiloxane^[1]: (a) C atom, (b) Si-O bond, (c) hollow of the cage and (d) Si atom.

Table S1 The adsorption of AO on polysiloxane^[2]

Adsorption site	Adsorption product	Adsorption energy (eV)
C	-CH ₂ -OH	-4.126
Si-O	-Si-O-O-Si-	-1.397
Hollow of the cage	O	-0.025
Si (Si-H)	-Si-OH	-6.391
AO	O ₂	-6.074

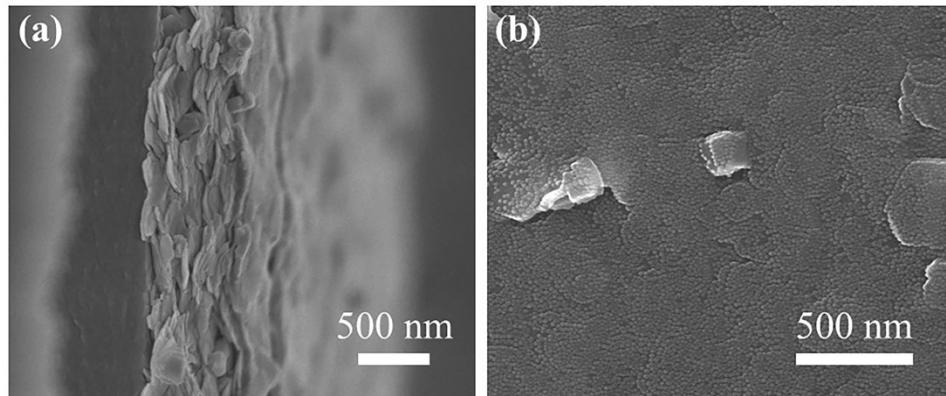


Fig. S2 SEM images of (a) cross-section and (b) surface of the L₁₁₀ sample after the atomic oxygen exposure test.

References

1. D.H. Tang, H.G. Li, H.Y. Gu, S.B. Lv, J.Y. Ma, Y.Z. Zhang and L.X. Song, *Surf. Coat. Technol.*, 2022, 447, 128840.