Full Title - The Title Should Be Bold and Centred (14pt)

Andreia Luisa da Rosa[1], Dominike Pacine[2], Daniel Souza, Renato Borges Pontes and Thomas Frauenheim[2]

[1]*Universidade Federal de Goiás, Campus Samambaia, 74690-900, Goiânia, Goiás, Brazil*
Instituto Federal de Educação, Ciência e Tecnologia de Goiás, Campus Jataí. 75804-714 Jataí, Goiás, Brazil

[2]*BCCMS, University of Bremen, Germany*

andreialuisa@ufg.br

Abstract

We carried out first-principles density functional theory calculations of hydrogen and oxygen adsorption and diffusion on subnanometer MoS nanowires. The nanowires are robust against adsorption of hydrogen. On the other hand, interaction with oxygen shows that the nanowires can oxidize with a small barrier. Our results open the path for understanding the behavior of MoS nanowires under realistic environment.

References

[1] M. Kendjy, A. L. da Rosa and Th. Frauenheim, J. Phys.: Condens. Matter 34 044005 (2022)
[2] F. B. de Oliveira, E. N. Lima, A. L. da Rosa, M. C. da Silva and Th. Frauenheim, Phys. Chem. Chem. Phys. 22, 22055 (2020)
[3] A .L da Rosa, E. N. Lima, M. Chagas da Silva, R. B. Pontes, J. S. De Almeida and Th. Frauenheim, The Journal of Physical Chemistry C 124 (21), 11708 (2020)
[5] D. Pacine, D. F. Souza, A. L. da Rosa, R. B. Pontes and Th. Frauenheim, https://arxiv.org/abs/2206.06342

Figures

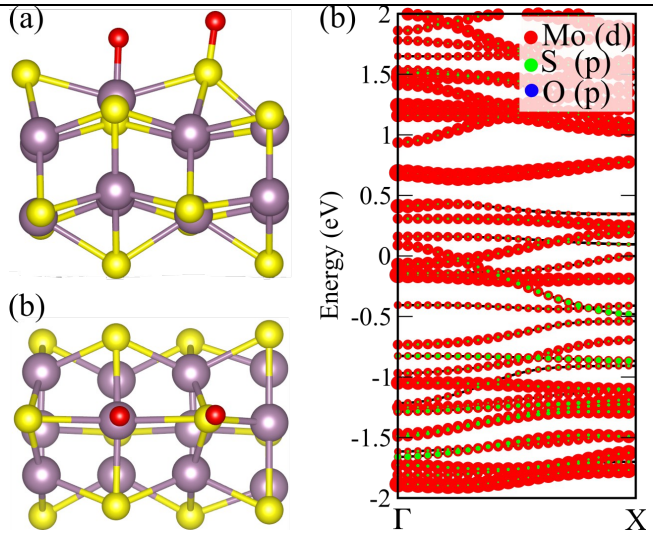

Figure 1: (a) and (b) Relaxed geometry and (c) electronic band structure of an oxygen molecule on MoS nanowires.