Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Monolayers of MoS2 and WS2 as oxidation protective nanocoating materials HUSEYIN SENER SEN, ENGIN DURGUN, UNAM - Bilkent University, HASAN SAHIN, FRANCOIS PEETERS, University of Antwerp — First-principles simulation techniques are employed to analyse the interaction of oxygen with MoS_2 and WS_2 monolayers. Our calculations show that while oxygen atoms are strongly bound on top of sulphur atoms, oxygen molecule only weakly interact with the system. The penetration of oxygen atom and molecule through MoS_2 monolayer require a very high energy barrier indicating that MoS_2 can serve as protective layer from oxidation. Not only ideal structures but also possible defect formations are considered and penetration/diffusion barriers of oxygen are calculated for each case. The study is extended for WS_2 as well, and obtained results are compared. Our predictions indicate that ideal and/or defected MoS_2 and WS_2 monolayers can improve the oxidation and corrosion-resistance of the covered surface and can be used as an efficient nanocoating material.

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Date submitted: 15 Nov 2013 Electronic form version 1.4