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Computational Modelling Studies of PtS surfaces

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Abstract content
   (Max 300 words)
Formatting &
Special chars

Precious metal sulphides such as PtS and PdS are major compounds occurring in the Pt and Pd ores, and play an important role as catalyst in the petroleum refining industry. In our previous work, the PtS and PdS minerals were investigated using density functional methods within planewave pseudopotential methods and predicted stability of PtS, Pt_{12.5}Pd_{37.5}S₅₀ and PdS phases. The current study is based on the surface properties of PtS and their interaction with oxygen and water molecules. It was found that the (101) surface displayed the lowest energy, hence is the most stable. Interestingly, the adsorption of oxygen show preferential to Pt atom, whereas with hydration of the surface gives a non-spontaneous reaction.

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MSc

Main supervisor (name and email)
and his / her institution

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