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First principle study of Xanthate and Diethyldithiophosphate adsorption on PtS (010) surface

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Abstract content
 (Max 300 words)
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Platinum surface has been studied extensively in recent years to improve the fundamental understanding of the mechanism of oxidation reaction on metal surfaces. These surfaces have a wide scientific and technological interest, particularly because of their catalytic properties. Density functional theory (DFT) method has been employed to study the surface properties of Platinum sulphide mineral PtS (010) and their interaction with xanthate and diethyldithiophosphate. It was noted that the adsorption energy of SEX is more exothermic compared to EX and IBX is more exothermic compared to SIBX. Furthermore, the adsorption energy of DEDTP shows that it is high in selectivity.

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Yes

Level for award (Hons, MSc, PhD, N/A)?

MSc

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

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