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Interaction of methanoic acid with arsenopyrite (001) and sperrylite (100) surfaces: A DFT-D and atomistic simulations studies

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The study of the surface chemical behaviour of sulphides and arsenides is very crucial in the field of mineral processing and ore beneficiation. The dispersion-corrected density functional theory (DFT-D) and atomistic simulations were employed to investigate the adsorption behaviour and mechanism of methanoic acid on arsenopyrite (001) and sperrylite (100) surfaces. It was found that methanoic acid preferred to adsorb on the Fe and Pt sites than As and/or S atoms on arsenopyrite and sperrylite, respectively. The adsorption energy of methanoic acid on arsenopyrite was −62.52 kJ/mol, while the adsorption on sperrylite gave −20.40 kJ/mol from DFT-D simulations. It was clear that methanoic acid preferred the arsenopyrite than sperrylite mineral. This study predicted that it is easy to remove limescale such as calcium carbonate (CaCO3) on sperrylite without methanoic acid adsorbing to some extent on the surface, while on arsenopyrite the methanoic acid may be adsorbed. Similar findings were obtained from atomistic simulations and therefore these methods can be used concurrently to understand surface reactivity of these minerals.

Apply to be considered for a student ; award (Yes / No)?

Yes

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

MSc

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