First-principles molecular modelling applied to the flotation of iron ores

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ABSTRACT

Flotation is the most used mineral separation technique worldwide, processing several billion tonnes of ore per year, including hematite and magnetite ores. Based on physical-chemical properties of mineral surfaces, flotation aims at selectively adsorbing molecules that render mineral surfaces either hydrophobic or hydrophilic, known as collectors and depressants, respectively. Hydrophobic particles are then recovered in the froth by the injection of gas bubbles travelling up in the cell and attaching the hydrophobic particles.

Static Density Functional Theory and Ab initio Molecular Dynamics simulations currently represent powerful tools for different applications in material sciences, like catalysis or depollution [1,2]. They have recently been successfully applied in the flotation area, with an increasing number of publications dealing with this topic every year [3].

These tools provide crucial information on the adsorption mechanisms of reagents on mineral surfaces, key step in the flotation process. For instance, Ab Initio Molecular Dynamics simulations were associated with infrared spectroscopy to unravel the until-then controversial adsorption mechanisms of fatty acids on fluorite [4]. A similar work will be applied on other minerals like kaolinite or magnetite, which are involved in the iron recovery. [5]. A better understanding of the adsorption mechanisms of flotation reagents, provided by molecular simulations, will help to finely tune the amounts of reagents [5] and lead to the development of new reagents formulations.

Overall, these tools allow proposing practical and industrial solutions to improve the flotation process, which will undoubtedly help the mining industry to face the challenge of the grade decrease and mineralogical complexness increase in ores.

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