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A DFT novel study on acidic and neutral arsenate and enoic/enoate collectors adsorption on spodumene and feldspar mineral surfaces

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Spodumene (LiAlSi2O6) is a significant source of lithium that is widely used for commercial purposes such as in batteries, particularly for electric vehicles. In natural ore deposits, spodumene is commonly found alongside feldspar as the common gangue mineral. Density functional theory computational method was used in this study to investigate the interaction of arsenate and enoate/enoic collectors on both minerals at acidic and neutral simulated conditions. The minerals most stable surface had surface energies of 0.71 J/m². for Spodumene (110) surface, while the feldspar (001) surface had 0.831 J/m². The collectors, hydrogen butyl arsenate, sodium butyl arsenate, (E)-4-octenoic acid and sodium (E)-4-octenoate were adsorbed on the (110) surface of spodumene and (001) surface of feldspar. The butyl sodium arsenate molecule preferred to bind with the Al atoms on the spodumene surface and gave the most exothermic adsorption energy of -630,38 kJ/mol. For feldspar, the butyl hydrogen arsenate gave the adsorption energy of -335,41 kJ/mol. This showed that the arsenate collectors bind stronger than the enoate and enoic acids which are similar to oleic acids. Moreover, the arsenate prefers to bind strong with spodumene than feldspar, which suggest that the collector is feasible to separation of these minerals. Furthermore, spodumene prefers to bind strong with arsenate under neutral condition, while the feldspar bond strong at acidic. Therefore, the separation of spodumene from feldspar may be achieved using arsenate collector under neutral conditions.

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