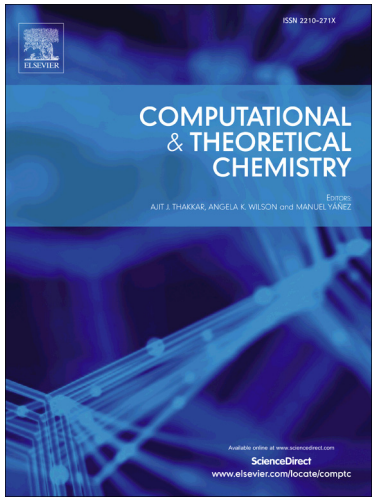

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Computational Modelling of Interactions between Gold Complexes and Silicates

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Abstract

The interactions of gold complexes including gold chloro-hydroxy species, gold thiosulphate and gold thiourea, with protonated and deprotonated silicate monomers, are studied using density functional theory (DFT) methods. The previously published optimal geometry of gold complexes is used here, together with the geometry of silica monomers that is optimised and compared with experimental and available theoretical data. COSMO (COnductor like Screening Model) solvation simulation of different systems (for different pH and gold complexes) is also used to represent the surrounding aqueous environments. The interaction energy of gold complexes with silica species based on theoretical studies has been shown to correlate well with the extent of silica preg-robbing (sorption) per surface area of quartz determined experimentally. The ability of DFT to compute the interactions of different gold complexes involving significant relativistic effects, with other species, has been demonstrated in this study. This work allows us to explain and control the chemical processes which result in loss of gold from solution in hydrometallurgical extraction.

Keywords: Density functional theory; COSMO solvation; gold chloride; gold thiourea; gold thiosulphate; silicate

1. INTRODUCTION

Carbonaceous matter and sulphides are well known to adsorb gold from leaching solutions in a phenomenon known as preg-robbing [1]. The mechanism of interaction of gold complexes with ore constituents has been the subject of investigation over the last few decades [2], and it has more recently been demonstrated that silicates can also be highly problematic in causing preg-robbing. However, previous studies of preg-robbing have focused mainly on gold cyanide complexes in view of its dominant use in gold extraction, meaning that non-cyanide gold complexes have not received as much attention. With increasing community resistance to the use of cyanide, there is renewed