

Geochemical characteristics of heavy metals in soil profile from an old metalliferous mining area in China

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Factors affecting the geochemical behavior of HMs

Heavy metals (HMs) is a major concern due to its potentially adverse impacts on public health [1, 2]. In mining areas, the essential of the natural pedogenesis is the elemental recombination and migration [3]. However, the process can be greatly accelerated by human mining activities.

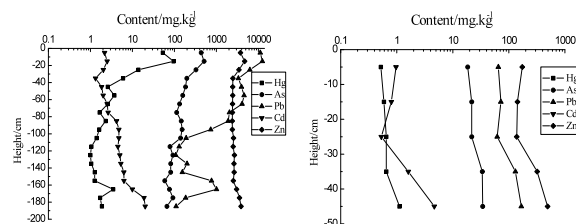


Figure 1: Vertical distribution of HMs in the soil profile. (Left-soil from mining area; Right-soil from control site)

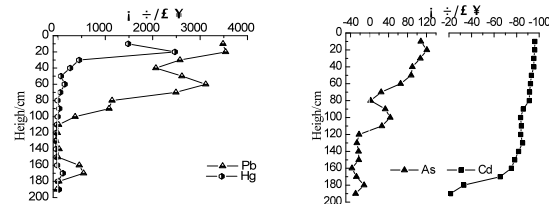


Figure 2: Migration ratio (Δ) of HMs in comparison with Fe.

Discussion of Results

The migration features of the major elements revealed that the soil from the mining area finished the primary process of chemical weathering characterized by leaching of Ca, and initiated the secondary process accompanying by leaching of K. Except the element Cd, other HMs such as Pb, Hg and As were enriched (Figure 2). It might be caused by both the pedogenesis and human mining activities. Extensive human mining activities made a major contribution to the accumulation of HMs in top soil.

- [1] Li *et al.* (2009) *Environ Geochem Health* **31**, 617-628. [2] Ji *et al.* (2009) *Acta Scientiae Circumstantiae* **29**, 1094-1102. [3] Chen *et al.* (2008) *J. Geogr. Sci.* **18**, 341-352.

Computational studies of structural, magnetic, and spectroscopic properties of actinide species

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The complicated electronic structure of actinide complexes leads to their versatility of chemical reactivity, spectral and magnetic properties, and dynamical behavior. We will show that first-principle computational chemistry modeling can be used as an effective tool to provide insight into these properties. Recent theoretical and spectroscopic studies indicate that variations of orbital character in bonding interactions are connected with differences in chemical reactivity. In this study, we applied density functional theory (DFT) to probe the electronic structure of the ground state of actinide complexes. We found that calculations provide a quantitatively accurate microscopic picture of the bonding interactions of the actinide-ligand bonds. Based on the understanding of fundamental bonding interactions, we will discuss the magnetic and dynamic properties. We found that time-dependent density functional theory (TD-DFT) correctly reproduces the experimental spectroscopic results, lending confidence to characterize the transition nature of excitations. These fundamental findings provide a solid foundation towards a more complete and accurate understanding of the physico-chemical properties of actinide complexes in the natural environment.

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