Assessment of heavy metal contamination in soils around Chinnaeru river sub-basin, Nalgonda District, India

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The concentration of heavy metals such as As, Ba, Co, Cr, Cu, Ni, Pb, Rb, Sr, V, Y, Zn and Zr were studied in soils to understand metal contamination due to agriculture and geogenic activities in Chinnaeru river basin, Nalgonda district, India. This area is affected by the geogenic fluoride contamination. The contamination of the soils was assessed on the basis of geoaccumulation index, enrichment factor (EF), contamination factor and degree of contamination. Forty four soil samples were collected from the agricultural field from the study area from top 10-50 cm layer of soil. Soil samples were analyzed for heavy metals by using X-ray fluorescence spectrometer. Data revealed that, soils in the study area are significantly contaminated, showing high level of toxic elements than normal distribution. The ranges of concentration of Ba (370-1710 mg/kg), Cr (8.7-543 mg/kg), Cu (7.7-96.6 mg/kg), Ni (5.4-168 mg/kg), Rb (29.6-223 mg/kg), Sr (134-438 mg/kg), Zr (141.2-8232 mg/kg) and Zn (29-478 mg/kg). The concentration of other elements was similar to the levels in the earth's crust or pointed to metal depletion in the soil (EF<1). The high EFs for some heavy metals obtained in soil samples show that there is a considerable heavy metal pollution, which could be due to excessive use of fertilizers and pesticides used for agricultural or may be due to geogenic activities in the area. A contamination site poses significant environmental hazards for terrestrial and aquatic ecosystems. They are important sources of pollution and may results in ecotoxicological effects on terrestrial, groundwater and aquatic ecosystems.

Influence of interfacial water structure on surface protonation and ion adsorption at metal oxide surfaces

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The overall goal of our research is to quantitatively link experimental and computational results to elucidate the atomic scale structure and dynamics of aqueous solutions at metal oxide surfaces and to link these atomistic interfacial properties with their macroscopic manifestations. Most of our efforts have been directed toward the isostructural oxides rutile (TiO_2) and cassitertite (SnO_2). The surfaces of these oxides (primarily the 110 face) have been probed by X-ray and neutron scattering, second harmonic generation, pH and zeta potential titrations, and ab initio and classical MD. In total, these techniques reveal a fairly consistent picture of interfacial water structure and cation binding. Directly bound water molecules are more tightly held at the cassiterite 110 surface than rutile 110 surface, and this difference helps account for the observed differences in surface protonation and ion binding exhibited by these oxides.

This research has been largely supported by the Division of Chemical Sciences, Geosciences and Biosciences, Office of Basic Energy Sciences, U.S. Deparment of Energy.