Hydro and pedogeochemistry in relation to landuse/landcover in Mungi village, Medak District, Andhra Pradesh, India

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The study area Mungi village forms a part of deccan basalt terrain where mostly the soils are laterites. Lot of inorganic fertilizers is being used in the agricultural fields thus causing possible contamination in soils and groundwater. Soil and groundwater contamination by heavy metal ions is one of the most serious environmental problems. Thus keeping this fact twenty nine groundwater and twenty four soil samples have been analyzed using Perkin Elmer Sciex ELAN DRC II ICP-MS. In the groundwater samples Pb ranged between 0.01 and 13.31μg/l with an average concentration of 1.82 μg/l the permissible limit of 10 μg/l. Ni contents ranged between 1.76 μg/l and 393.14 μg/l with an average of 38.29 μg/l which exceeds the permissible limit of 20 μg/l. As ranged between 0.09 μg/l and 2.42 μg/l with an average of 0.40 μg/l this is within the permissible limit of 10 μg/l. Zn ranged between 4.79 μg/l and 204.09 μg/l with an average of 33.68 μg/l. Cd ranged between 0.005 μg/l to 0.49 μg/l with an average of 0.06 μg/l this is within the permissible limit of 3 μg/l.

With regard to the soil concentration Ni ranged between 32.92 mg/kg and 79.90 mg/kg with an average of 44.30 mg/kg. Pb ranged between 5.22 mg/kg and 14.45 mg/kg with an average of 10.21 mg/kg. Zn ranged between 124.42 mg/kg and 196.14 mg/kg with an average of 161.05 mg/kg. Co ranged between 29.64 mg/kg and 72.28 mg/kg with an average of 46 mg/kg.

Electronic structure of Ti, Zr, Hf and Sn containing garnets – Materials for immobilization of actinides

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Garnet, $A_3B_2X_3O_{12}$, have recently been considered as a candidate for actinide-bearing host matrices [1-3]. The presence of three different cation sites (A, B, and X), permits the incorporation of numerous elements into the structure. This not only gives rise to a large variety of naturally-occuring garnets, but also opens up the possibility of synthesizing artificial actinide-bearing phases with garnet structure. Present efforts are focused on structures that are derivatives of the fluorite structure, e.g. pyrochlore [1-4]. Garnets with high levels of Zr and Ti, such as kimzeyite and schorlomite have been found in nature, and their synthetic analogues have been ivestigated experimentally as nuclear waste form materials [4]. In order to potential of garnet to incorporate actinides, it is crucial to obtain a basic theoretical understanding of the bonding and electronic structure.

We have investigated the crystal structure, nature of interatomic bondings, and electronic structure of Ca_3 (Ti, Zr, Hf, Sn)$_2$Fe$_2$SiO$_{12}$ garnet, using first-principles calculations within the density functional theory (DFT). The calculated equilibrium lattice parameters and the interatomic distances are close to the available experimental values, with a slight overestimation due to the generalized gradient approximation (GGA) used in our calculations. The theoretical total density of states (DOS) and its projections onto the atomic orbitals are presented and analyzed for different values of the on-site Coulomb interaction (Hubbard *U*) within the Fe *d* states. In order to quantify the strength of the interatomic bonds, we have performed Bader analysis of the charge density. The result of this analysis provides insight into the relative radiation resistance of garnet as a function of composition.

[1] Omel'yananko *et al*. (2007) *Geol. Ore Dep*. **49**, 137-193. [2] Livshits (2008) *Geol. Ore Dep*. **50**, 470-480. [3] Laverov *et al*. (2010) *Geochem. International* **48**, 1-14. [4] Whittle *et al*. (2006) *J. Solid State Chem*. **180**, 758-791. [5] Utsunomoiya *et al*. (2005) *J. Nucl. Mater*. **336**, 251-260.