# A thermodynamic entrapment model for the quantitative description of selenite coprecipitation with calcite

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The trace element Selenium is of environmental relevance as a nutriant as well as a toxic element for animal and human life. The long lived fission product $^{79}$Se is of special concern in the context of nuclear waste management.

A possible retention mechanism for selenite in natural environments is the structural incorporation of the trigonal pyramidal oxyanion $Se(IV)O_3^{2-}$ into the calcite structure.

EXAFS and polarization dependent EXAFS measurements confirm, in agreement with previous results [1], the structural incorporation of selenite in calcite and the substition of carbonate for selenite, leading to the formation of a $Ca(SeO_3)_X(CO_3)_{(1-X)}$ solid solution.

Selenite incorporation, quantified in coprecipitation experiments at surface controlled steady state conditions and low supersaturation, is much higher (partition coefficient, $D_{exp} = 0.015\pm0.012$) than expected according to DFT calculations and thermodynamic considerations ($D_{theo} = 2\cdot10^{-10}$).

To bridge the gap between experiment and theory we present a thermodynamic entrapment model based on the assumption, that experimental observations reflect preferential incorporation of selenite into the calcite surface and subsequent entrapment upon crystal growth, while bulk DFT calculation reflect the high strain induced upon incorporation of selenite into the bulk calcite structure.

DFT calculations confirm that surface incorporation is energetically more favourable than bulk incorporation. Batch type adsorption experiments at calcite equilibrium confirm the analogy between surface adsorption (ion-exchange [2]) and coprecipitation.

The observation of growth inhibition in aragonite to calcite recrystallization experiments in the presence of selenite in solution is interpreted as experimental evidence for the energetical difference between bulk and surface incorporation of selenite in calcite.

[1] Aurelio *et al Chem. Geol.* 270, **2010**, 249-256. [2] Cheng *et al Surf. Sci.* 283, **1997**, L690-L695

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# Tawlah Specialized Alkaline Granite Prospect, Midyan Region, Arabian Shield, Kingdom of Saudi Arabia: Petrology. Structural Implications and REEs-RM Characterization

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The Tawlah albite granites-quartz synites is one of promising sites of REE- Ta-Nb- bearing alkaline granites in the Midyan Suite, NW Arabian Shield. The granite-syenite association is a highly lecucratic, albite-rich rocks with accessory columbite-tantalite, thorite, monazite, allanite, xenotime, zircon and cassiterite. Ages of 577± 4 Ma (Hedge, 1985) were obtained from isotopic ratios of Sr and Nd by $^{143}$Nd/$^{144}$Nd and $^{87}$Sr/$^{86}$Sr method. The precision is sufficient to indicate that the albite granite is post-orogenic with respect to Najd orogeny. The Tawlah granite is divided into abite-granite (in major) and quartz-syenite (in part). The albite granite is more highly mineralized, has higher modal albite contents and higher Nb/Ta ratios, both in whole surface rocks and in drill hole samples.

On the structural point of view, the relationship between fault system and/or shear zones reported and mineral potential provides excellent and interesting evidences of its occurrence. Bearing in mind the Najd fault zone provides interesting evidences concerning the relationship between such faults and REEs-Nb-Ta-Th mineralization. Therefore, the distribution of mineralizations are closely related to the main trends; WNW-ESE, NW-SE and ENE. On the other hand, reactivation of NW Najd fault system has been affected by Teriary rift tectonics, leading to the development of mineralization in Tawlah alkaline granites.

On the basis of petrographic, mineralogical signature and geochemical interpretations, it is suggested that the albite granite-quartz syenite of Jabal Tawlah has a magmatic origin indicating post-orogenic overprinting of A-type granites. By analogy with other Nb-Ta-REEs –bearing granites, the sodic bulk composition of Tawlah granite can be explained by fluorine enrichment in the magma, but much of the magmatic fluorine was lost upon crystallization because the low CaO, $P_2O_5$ and $Al_2O_3$ contents of melt precluded fixation of F in crystalline phases.

In fact, the Tawlah alkaline granite prospect is considered to be a promising metallogenic site for REEs and Nb-Ta-Th, where its geologic environment, structural framework and tectonic setting are reasonable for achievement.

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