

Microfocus X ray and laser fluorescence, analytical and mapping techniques, on heterogeneous minerals

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Fluorescence is a highly sensitive phenomenon capable of detection at concentrations below PPM which is widely used. A recurring problem in mineralogical and petrological applications of fluorescence is that this sensitivity leads to the collected data representing a number of convoluted signals that make interpretation difficult. We present results from two complementary time resolved (TR) techniques Photo luminescence (PL) extensively used in biological applications as Fluorescence lifetime imaging microscopy. (FLIM) and TR X-ray Excited Optical Luminescence (XEOL) Results are presented from some obviously heterogeneous minerals and also examples from some with much less obvious heterogeneity. The (XEOL) is collected on the I18 microfocus beamline at the Diamond Light source. The system can be used to simultaneously collect X-ray Absorption spectra or X-ray fluorescence (XRF) and simultaneously collect (CW) (XEOL), or (TR) (XEOL). This enables the combination of very high sensitivity with accurate quantification. Analysing the different decay lifetimes and ratios for a spatially resolved point emissions $\sim 3/3$ micron. Allows us to deconvolute the complex fluorescent signal. CW XEOL spectral data from 200-900nm collected from the same spatial resolution allows us to compare identified features with the literature. We also discuss mapping capabilities in both (XRF) and (CW) (XEOL) as either a function of either wavelength or incident photon energy.

Fluorescence intensity and lifetime map (figure1) collected from a Polished section of Microcline from the Derry Township Quebec The map is $\sim 0.5\mu\text{m}$ square collected using a confocal (TR) multiphoton pulsed laser excitation

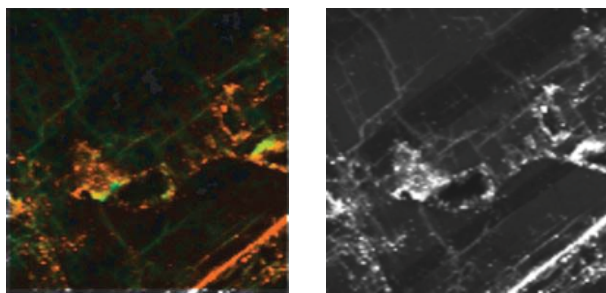


Figure 1: RHS luminescence intensity map LHS the same (TR) signal with deconvoluted lifetimes shown with false colour displaying the decay lifetime concentrations, deconvolution of complex multi component with signal red short lifetime blue long lifetime.

Accurate force fields built from ab-initio: the case of clays

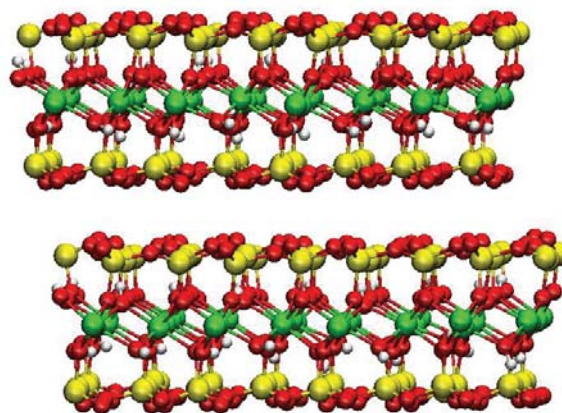
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Section heading

Molecular scale studies are essential for the prediction of sorption onto minerals such as clays, in particular in the context of the geological disposal of radioactive waste. The current state-of-the-art force field for clays, ClayFF [1], reproduces well several properties. However, it does not account for polarization, which is known to play an important role at solid liquid interface, in particular in influencing chemical specificity of cation sorption. We develop a polarisable force field for clays from DFT calculations, using on the one hand a force/dipole-fitting procedure, which provides a high degree of transferability [2], and on the other hand a systematic derivation using maximally localized Wannier functions [3].



Results and conclusion

We present here how the polarisable force field is constructed. We then demonstrate its validity by comparing structural properties to experimental data and to the current state-of-the-art non-polarisable force field ClayFF [1].

Figure 1: Snapshot of the pyrophyllite simulation box

[1] Cygan *et al.*, *J. Phys. Chem. B*, 108 (2004) 1255-1266.

[2] Jahn and Madden, *Phys. Earth Planet. Inter.*, 162 (2007), 129-139.

[3] B. Rotenberg *et al.*, *Phys. Rev Lett.*, 104 (2010).