Computational modeling of theoretical Illite fundamental particle using MDS

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Illite and smectite show special characteristic structure called 'interstratification' or 'mixed-layer'. They can be arrayed repeatedly with regular or random order. Our study focused on fundamental particle model theory. Interesting part of I/S interstratification is the polarity of fundamental particles. Our study is to evaluate if illite fundamental particle is appropriate to interpret illite/smectite interstratification, through Molecular Dynamics Simulation (MDS).

This study is still in beginning step, and we are doing number of calculations and geometry optimization of layer silicate models to build basic database for future study. The software used for modeling is Material Studio 2017 of Biovia$_{TM}$ and calculations were performed using CASTEP code based on Density Functional Theory (DFT). The electron exchange and calculation correlation was treated with Generalized Gradient Approximation – Perdew, Burke and Ernzerhof (GGA-PBE) functionals. Calculated models are 1M trans-cis illite and illite unitcell using different tetragonal substitution site. Trans-cis illite didn't show huge difference in stabilization energy, and small difference in XRD peak pattern. For Al-substituted illite model, pauling's rule was followed, and substitution at outer part of tetragonal showed smallest stabilization energy. Also, Al-substituted illite showed smaller stabilization energy than pure illite.

Further studies will be done using different calculation methods, and our next goal is to to consider convergence and find out the most proper method for further modeling, and find out the substitution mechanism of illite tetragonal site.

Keyword: Illite/Smectite, Interstratification, Geometry optimization, CASTEP, stabilization energy, fundamental particle