

## MS14-P32 | LAYER CHARGE INFLUENCE ON THE HYDRATION PROPERTIES OF SYNTHETIC NA-SATURATED SMECTITES

Vinci, Doriana (University of Bari, Bari, ITA)

Smectite hydration controls dynamical properties of interlayer cations and thus the fate and transport of water and pollutants. The influence of smectite crystal chemistry, and more especially of the amount and location of isomorphous substitutions, on smectite hydration has been largely documented over the last decade.[1] The influence of layer charge location, however, remains incompletely documented. The present study thus reports the influence of layer charge location on interlayer species organization by combining Powder X-Ray Diffraction (PXRD) profile modelling and Monte Carlo simulation in Grand Canonical ensemble. A set of octahedrally charged hectorites, with a common structural formula  $^{inter}[\text{Na}_x]^{oct}[\text{Mg}_{6.0-x}\text{Li}_x]^{tet}[\text{Si}_{8.0}]\text{O}_{20}(\text{OH})_4$  and a layer charge (x) varying from 0.8 to 1.6, was synthesized hydrothermally. Interlayer water contents were monitored as a function of relative humidity (RH) from H<sub>2</sub>O vapor (de)sorption isotherms. The evolution in proportions of both mono- and bi-hydrated layers was then determined from PXRD profile modeling as a function of RH. Then, Monte Carlo simulations were performed in the Grand Canonical ensemble to get additional details on the distribution of water molecules and charge-compensating cations within interlayers. Based on the comparison between octa- and tetrahedrally charged smectites [1] with contrasting layer charge, it is concluded that the evolution of layer-to-layer distance with the amount of layer charge differs for tetrahedrally and octahedrally charged smectites.

[1] Ferrage, E.; Lanson B.; Michot, L.J.; Robert J.L. (2010) Journal of Physical Chemistry C, 114: 4515-4526.