Capabilities of the MUltiSIte Model for Prediction of Isoelectric Points of Complex Minerals

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The isoelectric point of a mineral surface is a key parameter for the reactivity in terms of ion adsorption and colloidal stability. It results from the (de)protonation reactions of the hydroxyl sites present on the surface, which depend on pH according to their acidity constants. MUltiSIte Model [1] gives the possibility to calculate the value of these constants for each surface group, based on crystallographic data (atomic structure of each faces exposed to water). For simple oxides, this model succeeded in predicting the surface charging, and therefore the point of zero charge. However, its application to complex oxides has been little considered. We have applied this approach to predict the isoelectric point of lamellar materials of composition $Mn^{III}_xMn^{IV}_yO_z$ and $Co^{III}_xCo^{IV}_yO_z$, as well as that of particles formed by the stacking of these lamellae [2]. This result is an interesting way for optimizing the synthesis of these materials, and a validation of the MUSIC model for complex compounds.

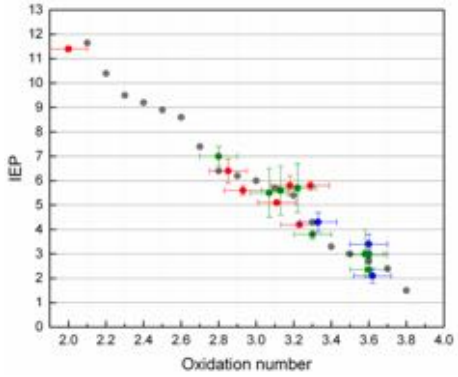

Fig. 1. Comparison of IEP values from calculation (grey dots) and experiments (color dots with error bars) for several solids with different mean oxidation numbers of the metal

[1] Hiemstra & Van Riemsdijk (1996), *J. Colloid Interface Sci.* 179, 488-508.

[2] Tang, Giaume, Guerlou-Demourgues, Lefèvre & Barboux (2018), *Langmuir* 34, 6670-6677.