Optimized molecular structures for nanokaolinite dehydration and dehydroxylation toward the formation of nanometakaolinite [dataset]

Authors: Robert K. Szilagyi and Attila Taborosi

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Description
The data depository contains XYZ atomic positional coordinates for all relevant structures to describe the dry-grinding, mechanochemical activation of nanokaolinite. During this process the kaolinite undergo dehydration, followed by edge dehydroxylation, dissociation of the surface trapped water, and finally dehydroxylation of the surface hydroxides. The overall five step procedure results in amorphous metakaolinite particle with highly activated surface sites. The theoretical results are in close correlation with SEM/TEM, FTIR, and TG/DTG experimental measurements.

Associated article
Zsirka B, Táborosi A, Szabó P, Szilagyi RK, Horvath E, Juzsakova T, Fertig D, Kristof J (2017) Surface Characterization of Mechanochemically Modified Exfoliated Halloysite Nanoscrolls. Langmuir, 33(14), 3534-3547. https://doi.org/10.1021/acs.langmuir.6b04606

Dataset citation
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