

Theoretical Investigation of MgF₂ Surface Structure

October 27, 2011

Project leader: Prof. Dr. Beate Paulus
Project administrator: Dr. Carsten Müller

Depending on the conditions under which microcrystalline magnesium fluoride (MgF₂) is prepared it exposes different surfaces. Therefore, it can show both Lewis and Brønsted base sites due to O²⁻ and OH groups at the surfaces, and additionally Lewis acid sites due to incompletely coordinated Mg²⁺ sites. This versatility makes MgF₂ interesting for a number of technological applications. Applying the methodology of *surface thermodynamics* in combination with density functional theory (DFT) calculations, our aim is to investigate what surfaces are exposed depending on the partial pressure of HF and H₂O above the surface and how these surfaces are terminated. Based on these results, the shape of MgF₂ microcrystallites can be simulated using Wulff construction and the most prominent facets will be probed for active sites by adsorption of carbon monoxide (CO), nitrous oxide (N₂O) and ammonia (NH₃).