Title: MgO Dissolution: A Model for Liquid-Solid Interface Reactions

Keywords: nanopowders, synthesis, morphology, crystal structure, phase transformation, dissolution.

Scientific description: Reactions at liquid-solid interfaces play a crucial role in natural geological processes and catalysis, often involving hydrogenation or dehydrogenation of reaction species. The transformation of magnesium oxide (MgO) into brucite (Mg(OH)2) serves as an excellent model for investigating dissolution phenomena. Our previous studies on MgO model nanopowders provided valuable first insights into effects during MgO dissolution processes (Baumann et al., Langmuir 2015, 31, 2770–2776). We found that particles must be sufficiently large to establish a protective surface layer that delays or inhibits dissolution. Additionally, large MgO cubes (> 100 nm) exhibit a dissolution-dependent shape transformation, with the (100), (110), and (111) planes becoming progressively apparent, subject to delayed dissolution. We propose a Master thesis to investigate the pH effect on MgO smoke dissolution. This study will involve synthesizing MgO powders through metal combustion within a glove box and immersing small quantities of these powders in liquid water and adjusting the pH between 4 and 10. The solutions will be analysed using X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and Diffuse Reflectance UV-visible Spectroscopy (DR UV-vis) over time. The experimental findings will be complemented by Density Functional Theory (DFT) simulations, and a parallel theoretical Master thesis could be envisaged. This research aims to enhance our understanding of liquid-solid interface reactions, with potential applications in geology, catalysis, and materials science.



Figure: Transformation of MgO particles upon their progressive dissolution in water (pH = 6.8). Adapted from *Phys. Chem. Chem. Phys.*, **2009**, 11, 2228.

Techniques/methods in use: synthesis via physical methods (evaporation based, metal combustion), SEM/TEM, XRD, DR UV-vis.

Applicant skills: any experience with the indicated experimental techniques will be considered as an advantage.

Industrial partnership: No (specify the company)

Internship supervisor(s) Slavica Stankic; <u>slavica.stankic@insp.jussieu.fr</u>; 0144274650 **Internship location**: 4, place Jussieu 75252 Cedex05 Paris. The tower 22, hall 22-12,5th floor.

Possibility for a Doctoral thesis: can be foreseen (specify if already financed).