

Poster presentation

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## Atomistic modelling of ion aggregation from solution and the self-organization of nanocrystals and nanocomposite biomaterials

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We present a recently developed simulation method for exploring the mechanisms of crystal nucleation from solution. By efficient tackling of the time-length scale problem, molecular dynamics simulations allow very detailed insights into the association of ions from solution and the development of structural motifs resulting in the nucleation of nanocrystals. Our studies of ionic self-organization include ripening reactions, such as proton transfer events and the interplay with growth-controlling molecules. The former issue is illustrated by the example of Zn<sup>2+</sup> and OH<sup>-</sup> association in ethanolic solution, condensation reactions leading to O<sup>2-</sup> ions and the nucleation of ZnO domains in the aggregate core. The interplay of ionic ordering and growth-controlling molecules is of particular interest for the investigation of composite materials. By the example of biomimetic apatite-collagen models, we demonstrate the design of crystal motifs induced by ion association to the protein fibers.

### References

1. Kawska A, Brickmann J, Kniep R, Hochrein O, Zahn D: *J Chem Phys* 2006, **124**:24513.
2. Tlatlik H, Simon P, Kawska A, Zahn D, Kniep R: *Angew Chem Int Ed* 2006, **45**:1905.
3. Kawska A, Hochrein O, Brickmann J, Kniep R, Zahn D: *Angew Chem Int Ed* 2008, **120**:5060.
4. Zahn D, Hochrein O, Kawska A, Brickmann J, Kniep R: *J Mater Sci* 2007, **42**:8966.
5. Kawska A, Duchstein P, Hochrein O, Zahn D: *Nanoletters* in press. (asap article online).