Molecular Modeling of ZnO Nanoparticle Nucleation: from pre-nucleation clusters to functionalized particles

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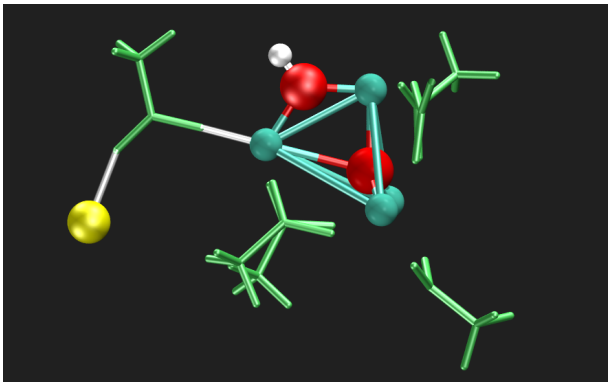

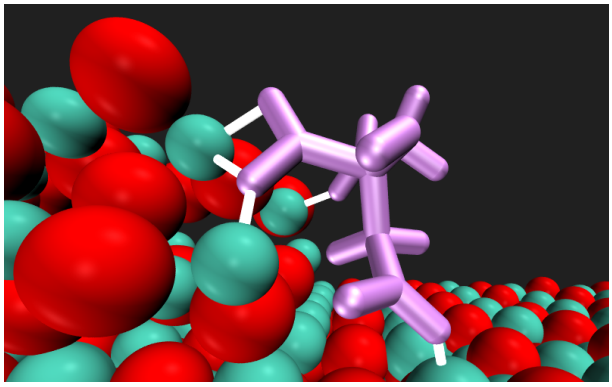

We demonstrate the molecular modeling of ion cluster formation, ripening reactions, nucleation and growth of zinc oxide nanomaterials. Furthermore molecular mechanisms of growth control, stabilization and functionalization by surfactants are elaborated. This is aiming at a fundamental understanding needed for the guided formation of nanostructures with tailor-made properties. Our simulation scheme (Kawska-Zahn method [1,2]) allows to explore the evolution of a forming aggregate ion-by-ion. In doing so, the method combines Molecular Dynamics, Monte-Carlo and quantum/classical modeling to tackle the time/length-scale problem inherent to crystallization from solution [3]. Mechanistic insights are presented for the very initial steps of pre-nucleation cluster formation of Zn^{2+},OH^- and $Zn_4O(Ac)_6$ precursors (figure 1). Moreover, cluster ripening and nucleation of $ZnO/Zn(OH)_2$ core/shell nanoparticles are shown [4]. Subsequent stages of particle growth are explored for various crystal surfaces, along with the association of surfactants (figure 2). Based on such detailed information, scale-up models are formulated and applied for the investigation of nanoparticle solvation and stabilization in colloidal solutions.

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[3] J. Anwar, D. Zahn, *Angew. Chem. Int. Ed.*, **2011**, 50, 1996.
[4] A. Kawska, P. Duchstein, O. Hochrein, D. Zahn, *Nano Letters*, **2008**, 8, 2336.