The Role of Capping agents in nano material synthesis - some thoughts

B.Viswanathan
National Centre for Catalysis Research
Indian Institute of Technology Madras, Chennai 600 036

14th April, 2013

Abstract

The Presentation examines the various types of capping agents normally employed in the preparation of Nano particles. The purpose of this presentation is to examine what factors control the size shape of nano materials synthesized and what is the role of the capping agents in these functions. The need for both hydrophilic and hydrophobic character present in capping agents is brought out. The association of capping agent with the nano materials decide the size, shape and also number of species since with the capping agents the material reaches a solubility limit and hence get out of the dissolved state to a sol state.

1 Introduction

It is known that some reagents with particular functional groups are employed in the synthesis of nano materials. They are usually termed as capping agents. They are in a conventional sense contain some functional groups which can ligate the metal nano particles if the nano material synthesized is metal nano state. There are always questions regarding the various reagents that are employed in the preparation of nano materials. One of them is this capping agents which are either carboxylate groups, or contain functional groups like amino groups and some coordinating atoms like the hetero atoms which can bind to the metal nano particles. The possible propositions for which one may like to find answers are
(i) what should be the nature of the substances that can be termed as capping agents?
(ii) What type of functionalities in capping agents are most often preferred and why?
(iii) Does the capping agents only aid in nucleation and its growth or do they also responsible the shape and size of the nano particles formed.
These and many other questions stand when one tries to probe the capping agents. In this short write up it is our intention to throw some thoughts on these questions and provide somewhat partial answers to them.
It has been recognized that the capping agents should contain some functional groups (if they were to be used for the preparation of metal nano particles)

and these functional groups normally contain some hetero atoms and thus impart some hydrophilic character to the molecule. However if the capping agents are totally hydrophilic then they will be in the dissolved state in the solvent system employed for the synthesis of nano materials. Therefore the capping agents should also contain some hydrophobic moiety like alkyls groups and thus the capping agents employed must have predominant hydrophobic character but with some fraction of hydrophilic character so that the capping agents will have necessary and solubility in the solvent system empolyed for the synthesis. This stipulation of the characteristics of capping agents places one restriction on the nature of capping agents that is the species must have predominant hydrophobic character with sufficient hydrophilic character to be able to be present in solution so that they can hook on to the nano material nuclei that will be formed. The type of functinalities in the capping agents are those that contain functional groups with hetero atoms. These functional groups impart sufficient ionicity in the molecule so that they could hook on to the nano metals that are formed. If the ionicity imparted to the molecule by the functional hetero atom containing species is large enough they will remain mostly in the solvent medium in which the nano material is prepared and the quantities of capping agents required for the nano material preparation will also be higher. Therefore the total hydrophilic character in the capping agent should be optimum and hydrophobicity should be predominant so that the cappling molecules can hook on to the nano materials as they nucleate and grow.It is therefore possible that capping agents to some extent the size of the nano particles that are obtained from the preparation solution. When the capping agent hooks on to the metal nano particles of certain size, they reach solubility limit, since the net charge on the metal particle is now controlled by the hooked up capping agent. If in addition to these species in solution if some support material were also to be present then the activity coefficient of of the dissolved species will be controlled by the ionic strength in the medium and thus the particle size will depend what type of support is employed and its solubility in the medium in which the nano material is prepared. One can rationalize based on the suport which will increase the ionic strength of the medium used for the synthesis and thus predict that on those supports with a given concentration of the species, the nano material synthesized will have the small or bigger size. Regarding the third question if the capping agent controls the shape of the nanoparticles formed, the reflection appear to be positive though the author does not have any concrete evidence from literture or any rational to propose. However, since the nature of the capping agent and also its hooking on the growing nanomaterials decide what will be the appropriate site in the growing nano material the capping agent will hook up and thus it decides the shape of the nano materials formed. At this stage, the material presented in this write up appears to be only proposals and the validity of these statements require solid examples and this will be taken up in a next write up.

1.1 Acknowledgement

The concepts developed in this article stem from one of the weekly discussion we have in our centre and grateful thanks to these research scholars who have stimulated this kind of discussion.