A rapid estimation of the average core-shell nanoparticle size by calcination and modeling

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Nanoparticles have a large area of interest due to the structure – property relations that have led to remarkable applications. In the characterization of the nanoparticles, the size represents a critical part of measurement, currently made using various techniques as TEM, BET or the motion of the particle in response to some force, such as gravity, centrifugal force, Brownian motion or electrostatic force.

The aim of this communication is to present a less costly and easy hand estimation of the average size of the nanoparticles having the hard core – shell structure using apparently two different procedures, and namely an experimental one (calcination) and another theoretical(molecular modeling).

The method is based on the assumption that the ratio between M_2/M_1 masses from the sample (M_2 is the lost mass and M_1 = M-M_2 the mas remained after calcination) is equal to the m_2/m_1 ratio of the core – shell masses from the "average size " nanoparticle

$$q = \frac{M2}{M1} = \frac{m2}{m1} \text{ and hence } q' = q\frac{\rho 1}{\rho 2} = \frac{M_2}{M - M_2}\frac{\rho 1}{\rho 2},$$

where ρ_1 is the core density and ρ_2 the density of the molecules situated in the shell.

This ratio and the modeling of the shell of the coated core allows us to obtain an expression for the average diameter of the nanoparticle:

$$D = 2d\frac{(q'+1)^{\frac{1}{3}}}{(q'+1)^{\frac{1}{3}} - 1}$$, where "*d*" is the diameter of the molecules from the shell.

The method has successfully been applied for five magnetite – aminoacid nanoparticles (aspartic acid, glutamic acid, proline, arginine and tryptophan), the estimated average size values being favourably compared with the corresponding TEM ones.