Theoretical Calculations

A very rough and approximate calculations to obtain:

- Calculation of the number of ZnO unit in each ZnO nanoparticle
- Calculation of the number of TDI per each ZnO nanoparticle
- Calculation of the relative surface of ZnO nanoparticle covered by TDI units

According to the diameter of the ZnO nanoparticles (25 nm), we can obtain the following information with numerical calculations:

Volume of sphere: V= 4/3 πr^3 , the Volume of each ZnO nanoparticle: 8181.2 nm^3

Surface area of a spherical ZnO nanoparticle: A= 4 πr^2 = 1963.5 nm^2

Regarding the bulk density of NP 5.6 g/cm^3 = 5.6 × 10^{-21} g/nm^3 and using: m=ρv the weight of each nanoparticle was obtained:

Weight of each NP 4.581 × 10^{-17} g

Weight of each ZnO unit 13.523 ×10^{-23} g

By dividing the mass of the particles per unit weight, the number of ZnO units in each ZnO nanoparticle can be obtained:

Number of ZnO units in each NP = 338700

And we know the percentage of nanoparticles in each sample using data from TGA,

For example in 1 g ZnO-TDI:

ZnO 0.889 g = 0.01092 mol ZnO units = 6.574 × 10^{21} unit ZnO = 1.941×10^{16} number of ZnO NP = 3.22 × 10^{-8} mol ZnO NP

TDI 0.111 g = 6.372 × 10^{-4} mol

TDI/ZnO NP= 19800 TDI for each ZnO NP

As a result, the substituents attached to ZnO nanoparticles can be very roughly calculated:

radii of Zn^{2+} in crystal 88 pm = 88 × 10^{-12} m = 0.088 nm [1]

radii of Zn^{2+} in crystal 125 pm = 125 × 10^{-12} m = 0.125 nm

Surface occupied by all TDI groups 3.14×0.125×0.125 ×19800= 971 nm^2

TDI occupied surface / total sphere surface 971/1963.5 = 0.495 or 49.5%

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[1] D. R. Lide, CRC Handbook of Chemistry and Physics, 90th Edition, 2010, CRC Press.