

# Cadmium Oxide (CdO) Smart Nano Particles, Nano Capsules and Nanoclusters Influence, Impression and Efficacy in Cancer Prevention, Prognosis, Diagnosis, Imaging, Screening, Treatment and Management under Synchrotron and Synchrocyclotron Radiations

Alireza Heidari<sup>1,2,3,4,\*</sup>, Margaret Hotz<sup>1,2,3</sup>, Nancy MacDonald<sup>1,2,3</sup>, Victoria Peterson<sup>1,2,3</sup>, Angela Caissutti<sup>1,2,3</sup>, Elizabeth Besana<sup>1,2,3</sup>, Jennifer Esposito<sup>1,2,3</sup>, Katrina Schmitt<sup>1,2,3</sup>, Ling-Yu Chan<sup>1,2,3</sup>, Francesca Sherwood<sup>1,2,3</sup>, Maria Henderson<sup>1,2,3</sup>, Jimmy Kimmel<sup>1,2,3</sup>

<sup>1</sup>Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA

<sup>2</sup>BioSpectroscopy Core Research Laboratory, California South University, 14731 Comet St. Irvine, CA 92604, USA

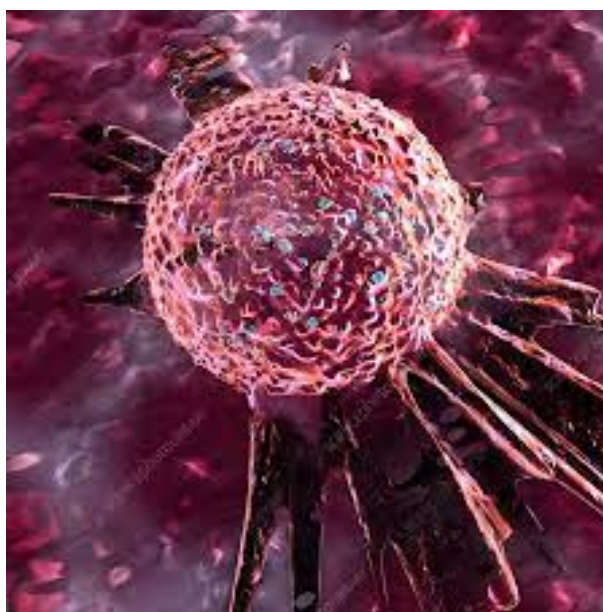
<sup>3</sup>Cancer Research Institute (CRI), California South University, 14731 Comet St. Irvine, CA 92604, USA

<sup>4</sup>American International Standards Institute, Irvine, CA 3800, USA

\*Corresponding author: [Scholar.Researcher.Scientist@gmail.com](mailto:Scholar.Researcher.Scientist@gmail.com)

Received July 20, 2021; Revised August 21, 2021; Accepted August 29, 2021

**Abstract** In the current research, the effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations is investigated. The calculation of thickness and optical constants of Cadmium Oxide (CdO) the effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations produced using sol-gel method over glassy medium through a single reflection spectrum is presented. To obtain an appropriate fit for reflection spectrum, the classic Drude-Lorentz model (Appendix A) for parametric di-electric function is used. The best fitting parameters are determined to simulate the reflection spectrum using Lovenberg-Marquardt optimization method. The simulated reflectivity from the derived optical constants and thickness are in good agreement with experimental results.



The effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations.

**Keywords:** structural, morphological, optical and electrical properties, Nanostructured cadmium Oxide (CdO), nano thin films, anti-cancer nano drug, cancer cells, tissues and tumors, synchrotron and synchrotron radiations

**Cite This Article:** Alireza Heidari, Margaret Hotz, Nancy MacDonald, Victoria Peterson, Angela Caissutti, Elizabeth Besana, Jennifer Esposito, Katrina Schmitt, Ling-Yu Chan, Francesca Sherwood, Maria Henderson, and Jimmy Kimmel, "Cadmium Oxide (CdO) Smart Nano Particles, Nano Capsules and Nanoclusters Influence, Impression and Efficacy in Cancer Prevention, Prognosis, Diagnosis, Imaging, Screening, Treatment and Management under Synchrotron and Synchrotron Radiations." *Journal of Materials Physics and Chemistry*, vol. 9, no. 2 (2021): 26-46. doi: 10.12691/jmpc-9-2-1.

## 1. Introduction

The effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrotron radiations is investigated. Cadmium Oxide (CdO) is a semi-conductor of type n which its 3d level is filling up [1-67] and it belongs to a group of smart materials that reacts to variations of temperature, electrical or magnetic fields and pressure. This oxide can be used as thin films for a wide range of applications including electrical and or optical-thermal switching tools and energy storing covers [67-103]. Therefore, determining optical constants (refractive coefficient, n, and extinction coefficient, k) of Cadmium Oxide (CdO) thin films is essential for designing optoelectronic and optical tools for producing optical covers and similar tools such as multilayer covers and filters [104-184]. The measured experimental parameters including optical reflectivity are used as a function of wavelength to determine optical parameters of thin layers [185-257]. For determining optical parameters, various physical models such as Kusch, Frouhi-Blumberg and Taw-Lorentz have been suggested to calculate refractive coefficient, n, and extinction coefficient, k. For any thin layer, an appropriate optical model should be selected and used for estimation of real and imaginary di-electric function according to its physical condition [258-313].

To do this, an initial guess is needed for parameters of di-electric function and thickness which is defined as a range regarding physical characteristics of thin film and the available results in the literature. In faculty of Chemistry, BioSpectroscopy Core Research Laboratory and Cancer Research Institute (CRI) at California South University, Irvine, California, USA, under similar conditions, Cadmium Oxide (CdO)-the effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrotron radiations are produced over glassy medium in sol-gel laboratory. Measurement of thin films are performed on four samples of Cadmium Oxide (CdO) as the effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrotron radiations with

mole ratio of 0.5, 1 and 1.5% of Cadmium Oxide (CdO) [314-467]. Simulation of experimental spectra are performed using a single reflection spectrum of thin films and through Drude-Lorentz physical model (Appendix A) in optimization process of Levenberg-Marquardt. Optical constants such as reflection coefficient, n, extinction coefficient, k, and layer thickness are simultaneously determined at wavelength of 400-1100 (nm).

## 2. Modeling, Simulation and Calculation Method

A usual method for describing optical constants of thin films is utilizing classic dispersion relationships based on di-electric function. One of the oldest and most applicable dispersion relationships is Drude-Lorentz di-electric equation (Appendix A) which is based on the interaction between light and material. This relationship is shown in Eq. (1):

$$\varepsilon = \varepsilon_{\infty} + \sum_{j=1}^n \frac{f_j E_{0j}^2}{E_{0j}^2 - E^2 + i\Gamma_j E} + \frac{E_p^2}{E^2 + iE_{\tau} E} \quad (1)$$

where  $\varepsilon_{\infty}$ ,  $f_j$ ,  $E_0$  and  $\Gamma_j$  are di-electric constant at high frequencies, resonance amplitude, power and resonance width-band which are recognized as the reason for damping. Damping is due to absorption process which includes transition between two states. The third term is related to Drude model (Appendix A).  $E_p$  is density of Plasma energy and  $E_{\tau}$  is incident energy [4]. The complex di-electric function as  $\varepsilon = \varepsilon_1 + i\varepsilon_2$  which describes the reaction of material with electromagnetic waves as a function of photon energy, E, or wavelength,  $\lambda$ , has a real part  $\varepsilon_1$  and an imaginary part  $\varepsilon_2$ . Real and imaginary parts of complex reflection coefficient, namely  $n(\lambda)$  and  $k(\lambda)$  are related to di-electric function as Eq. (2) [5]:

$$n(\lambda) = \left( \frac{\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2}}{2} \right)^{1/2}, \quad (2)$$

$$k(\lambda) = \left( \frac{-\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2}}{2} \right)^{1/2}$$

Reflection spectrum (R) of samples for normal incident is a function of film thickness d, medium reflection coefficient S, incident light wavelength  $\lambda$ , reflection coefficient  $n(\lambda)$  and extinction coefficient  $k(\lambda)$ .

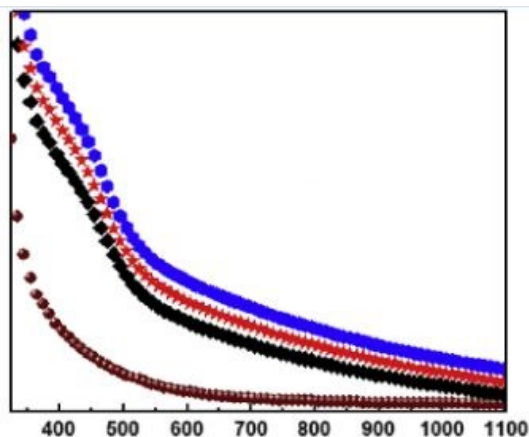
Simulation of the measured reflection data using optimization of objective function (O), which is the square of difference between the measured reflection spectrum and the calculated one, is defined as:

$$O = (\varepsilon_{\infty}, f, \Gamma, E_0, E_p, E_{\tau}, d) = \sum (R_{meas} - R_{calc})^2 \quad (3)$$

where,  $R_{meas}$  and  $R_{calc}$  are the measured and theoretical reflection spectrum, respectively. using the fitting parameters obtained from minimization of objective function, dispersion curves of reflection and extinction coefficients can be estimated.

### 3. Results and Discussion

The measured and simulated reflection spectra with fitting parameters of Cadmium Oxide (CdO)-the effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations at various concentrations of 0.5, 1 and 1.5%, named as a, b, and c, and the effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations sample, named as p, are shown in Figure 1 in wavelength range of 400-1100 (nm) (visible regions close to infrared) using Drude-Lorentz model (Appendix A) for air, film, medium, air system.



**Figure 1.** Results of simulating the reflection spectrum for Cadmium Oxide (CdO)-the effect of solution molarity on the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations at concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) non-doped.

Comparison of the results were shown that the sample containing 0.5% of Cd (sample a) has shown more reflectivity than samples containing 1% and 1.5% of Cadmium Oxide (CdO) (samples b and c). As can be seen in Figure 1, the reflection of thin films is decreased by increase in mole concentration of Cd to Cadmium Oxide (CdO). This reduction can be attributed to various reasons such as increasing roughness, increasing thickness and increasing the concentration of contaminant. The results of

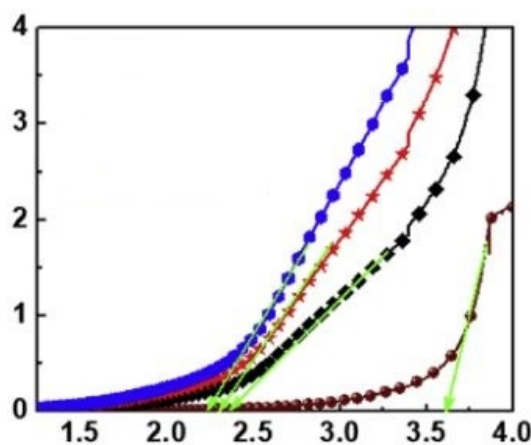
investigation about surface roughness using AFM (Atomic Force Microscopy) method confirms the increasing of roughness by increasing the concentration of Cd. Therefore, dispersion of incident light is increased in thin films. Variation of thickness of thin film by increasing the percentage of Cd is effective in variation of reflectivity of thin films which is due to sol viscosity. Changing the crystalline structure and chemical composition of thin films induced by penetration of Cd ions into the crystalline lattice of Cadmium Oxide (CdO) is another effective factor which leads to changing the reflection spectrum. The results of structural analysis using XRD (X-Ray Diffraction) confirms the tendency to be amorphous by increasing the concentration of contaminant.

The best fitting parameters obtained from optimization process and experimental data fitting are listed in Table 1.

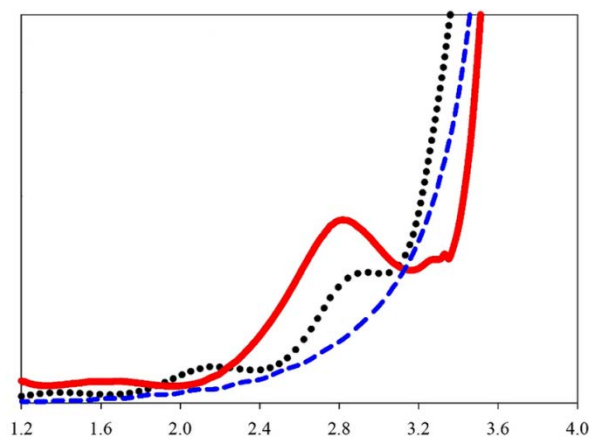
**Table 1. Fitting parameters of di-electric function of DL model**

Parameter	Pure	% 0.5 CdO	1% 1 CdO	% 1.5 CdO
$\varepsilon_{\infty}$	4.5	3.5	2.5	1.5
$E_p$	1.85	1.75	1.65	1.55
$E_{\tau}$	0.45	0.4	0.35	0.25
$f$	0.35	0.25	0.15	0.05
$E_0$	2.5	2.4	2.3	2.2
$\Gamma$	0.5	0.4	0.3	0.2
$d$ (nm)	200	300	400	500

As can be seen in Table 1, more increase in Cd leads to increase in  $\Gamma$ ,  $f$ ,  $E_0$  and  $d$  and decrease in other parameters as crystalline structure and inter-atom distance changes in lattice of Cadmium Oxide (CdO) thin film. According to [7],  $E_0$  in the range of 2.9-3.1 (eV) shows optical transition capacity band to displaced state of conducting band which according to the data of Table (1), it can be concluded that optical transition energy (gaff energy) increases with increase in Cd concentration. The calculation results of optical constants including reflection coefficient and extinction coefficient using the parameters of obtained di-electric function from the optimization process of thin films at various concentrations of Cadmium Oxide (CdO) as 0.5% (sample a), 1% (sample b) and 1.5% (sample c) are shown in Figure 2 and Figure 3, respectively.



**Figure 2.** Reflection coefficient of Cadmium Oxide (CdO) thin films with Cd concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) pure sample



**Figure 3.** Extinction coefficient of Cadmium Oxide (CdO) thin films with Cd concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) pure sample

As can be seen in Figure 2, reflection coefficient of samples at 500-1100 (nm) are the same and are decreased by increasing wavelength. By increasing the concentration of Cd, reflection coefficient is totally reduced which is in good agreement with the results related to variations of reflectivity in Figure 1 in which, increasing roughness leads to increase in dispersion and hence, reducing the amount of reflection spectrum. It can be seen in Figure 3 that  $k(\lambda)$  for two samples of p and a are of increasing rate at wavelength range of 400-500 (nm). Further, all samples are of decreasing rate at the range of 500-800 (nm). Totally,  $k(\lambda)$  is reduced by increase in Cd concentration. In other words, optical absorption is reduced in this range and the emerged peaks at extinction coefficient are in agreement with parameters of Drude-Lorentz (Appendix A) obtained from the optimization algorithm.

#### 4. Conclusions, Summary, Recommendations, Perspectives, Useful Suggestions and Future Studies

The results of optimization algorithm of Lovenberg-Marquardt with physical model of Drude-Lorentz (Appendix A) for determining optical constants of Cadmium Oxide (CdO)-the effect of solution molarity on

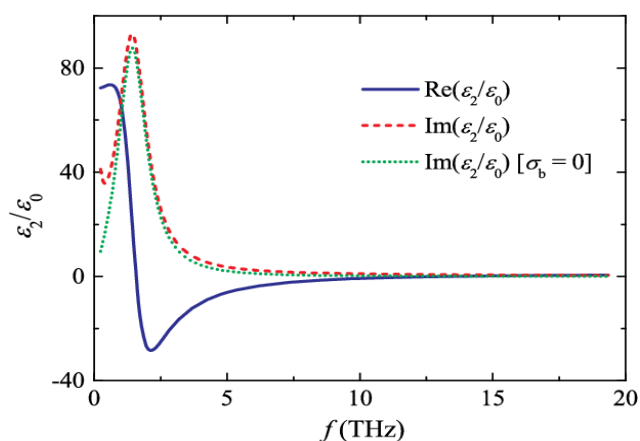
the structural, morphological, optical and electrical properties of nanostructured Cadmium Oxide (CdO) nano thin films as anti-cancer nano drug in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations produced using sol-gel method through a single reflection spectrum show that higher doping leads to lower reflectivity and reflection coefficient and also, leads to increase in thickness of thin layer.

#### Acknowledgements

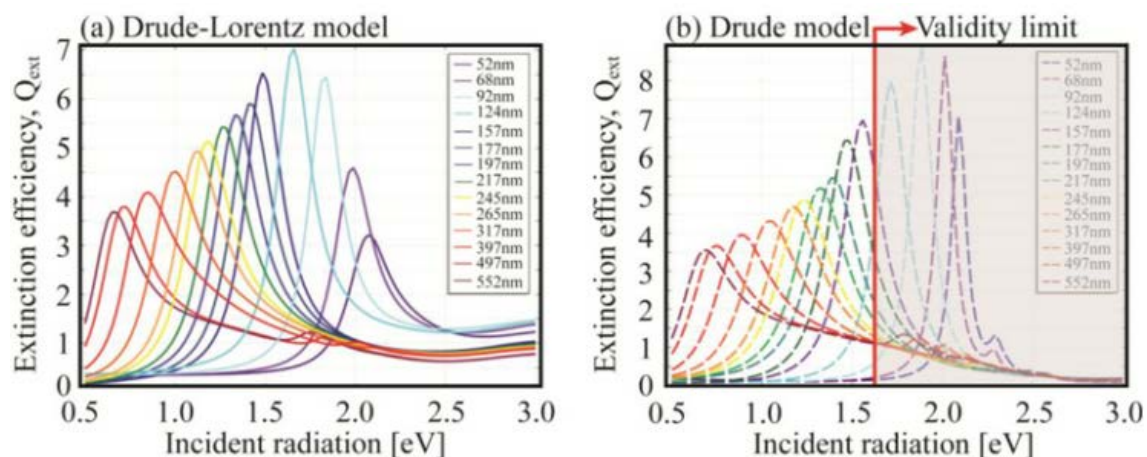
This study was supported by the Cancer Research Institute (CRI) Project of Scientific Instrument and Equipment Development, the National Natural Science Foundation of the United States, the International Joint BioSpectroscopy Core Research Laboratory Program supported by the California South University (CSU), and the Key project supported by the American International Standards Institute (AISI), Irvine, California, USA.

#### Appendix (A)

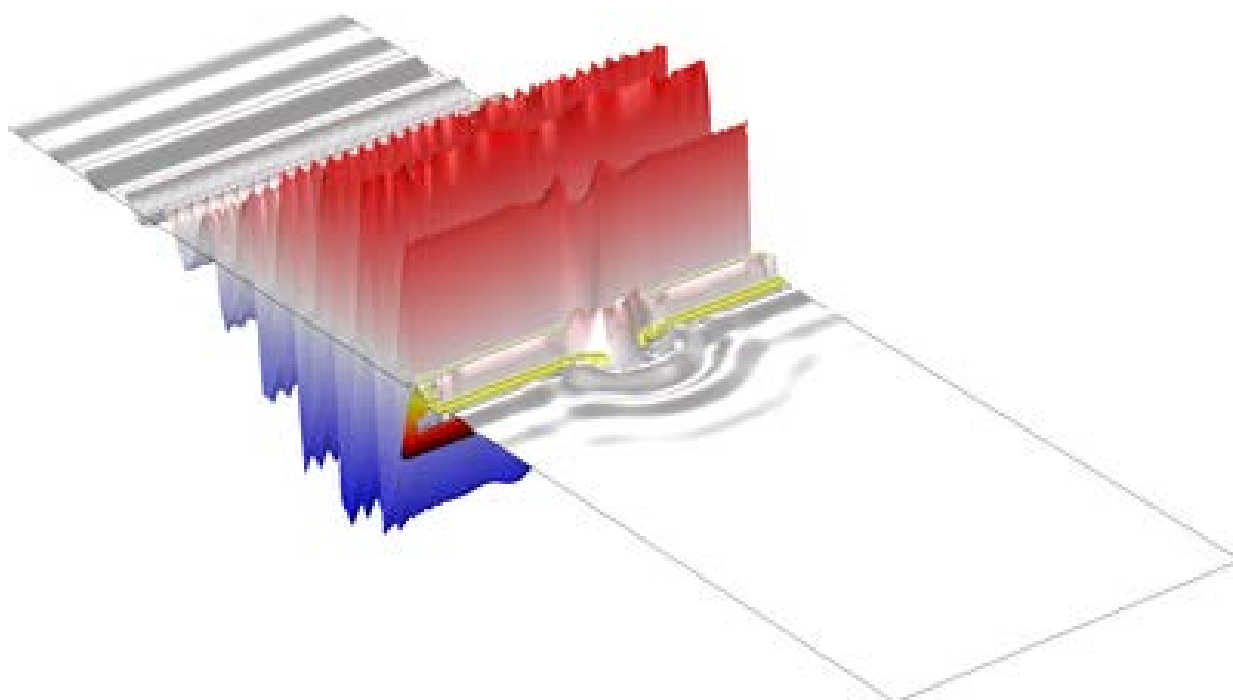
The Drude model of electrical conduction was proposed in 1900 by Paul Drude to explain the transport properties of electrons in materials (especially metals). Basically, Ohm's law was well established and stated that the current  $J$  and voltage  $V$  driving the current are related to the resistance  $R$  of the material. The inverse of the resistance is known as the conductance. When we consider a metal of unit length and unit cross sectional area, the conductance is known as the conductivity, which is the inverse of resistivity. The Drude model attempts to explain the resistivity of a conductor in terms of the scattering of electrons (the carriers of electricity) by the relatively immobile ions in the metal that act like obstructions to the flow of electrons. The model, which is an application of kinetic theory, assumes that the microscopic behavior of electrons in a solid may be treated classically and behaves much like a pinball machine, with a sea of constantly jittering electrons bouncing and re-bouncing off heavier, relatively immobile positive ions (Figure 4 - Figure 6) [468-488].



**Figure 4.** The Drude model, which is an application of kinetic theory, assumes that the microscopic behaviour of electrons in a solid may be treated classically and behaves much like a pinball machine, with a sea of constantly jittering electrons bouncing and re-bouncing off heavier, relatively immobile positive ions



**Figure 5.** The Drude model for Cadmium Oxide (CdO) smart nano particles, nano capsules and nanoclusters (a) before and (b) after synchrotron and synchrotron radiations



**Figure 6.** Simulation of the Drude model for Cadmium Oxide (CdO) smart nano particles, nano capsules and nanoclusters

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