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In-silico modeling of degrading nanomaterials as a novel approach for tumor therapy

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Here, our aim was to develop ZnO NMs with finely tuned degradation kinetics to maximize cancer-cell specific cell death. ZnO NMs were doped with different levels of Fe ions. Based on the intrinsic physicochemical properties of the NMs, quantitative nanostructure-activity relationship models were generated to define the dissolution rate and cell death of the different NMs and to generate an optimal formulation for toxic-by-design NMs that could selectively kill cancer cells while non-cancerous cells remained unaffected. Cytotoxicity of these NMs was tested in HeLa and KLN 205 (cancerous), MSC and BEAS-2B (non-cancerous) cell lines. Data revealed that low Fe-doping caused higher overall toxicity that was diminished as the Fe-doping increased. In-silico analysis revealed that 2% Fe-doped NMs were the most selective towards cancer cells, mainly through higher levels of oxidative stress and mitochondrial damage. These findings were confirmed in co-culture models where cancer cells were cultured with non-cancerous cells and exposed to the NMs. Thus, 2% Fe-doping, 25 µg/ml concentration, 8 hr. duration selectively killed cancer cells while the non-cancerous cells did not display significant toxicity. This was further evaluated in a syngeneic mouse model (DBA/2 mice with subcutaneous KLN 205 cells). Upon administration of pure, or 2 or 10% Fe-doped ZnO, the level of Zn^{2+} ions present in the tumor were inversely correlated to the Fe-doping level. The pure ZnO NMs were found to be toxic to the mice, while 10% Fe-doped NMs did not cause any toxicity nor a major therapeutic benefit. However, 2% Fe-doped NMs resulted in a clear reduction in tumor growth, without any negative effect on animal well-being. In conclusion, we have demonstrated that through controlled dissolution and in-silico modelling, NMs can be generated that cause selective cancer cell toxicity. This principle is likely generic and is easily applicable to other NM formulations.

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Electrical transport properties and dielectric response in Al doped NiO Nanostructures

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In this talk we have studied the electrical and transport properties of $Ni_{1-x}Al_xO$ (x = 0.00, 0.01, 0.03, 0.05) nanoparticles which have been synthesized through wet chemical route such as sol-gel method at 600^0C. The XRD patterns reveal that the NiO nanoparticles have cubic polycrystalline crystal structure with average crystallite size ranging from 18.20 to 9.54 nm which have been calculated through Debye-Sherrer and William Hall method. The morphology and size of the nanoparticles were also observed by Scanning electron microscopy (SEM) and transmission electron microscope (TEM) for pure and 5% Al doped NiO nanoparticles. We have studied the DC resistivity and activation energy of our samples using two probe measurements. In addition, dielectric response(τ), ac conductivity (σ_{ac}) loss tangent (tan δ) and impedance analysis have been carried out using LCR meter in the frequency range 75 kHz to 2 MHz with temperature range 50^0C– 400^0C . It has been observed that pure and Al doped NiO nanoparticles exhibit giant value of dielectric premitivity (10^3-10^4). The high value of dielectric constant of Al doped NiO nanoparticles depends on Al concentration and can be ascribed to the thermally activated and Maxwell–Wagner polarization mechanism.

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