Nanomedicine enables unique diagnostic and therapeutic capabilities to tackle problems in clinical medicine. The delivery of drugs, antigens, and imaging agents benefit from using nanotechnology-based carriers. However, from the entry of the therapeutic nanoparticle into the host’s blood circulation, the nanoparticle faces a long journey to its intended destination. During that journey, there are several barriers that need to be overcome. These hurdles are often neglected or disregarded in physiochemical evaluations of the future possibilities of nanotechnology to deliver agents to specific targets.

In this talk we report on our latest results on the interactions of nanoparticles with cellular membranes. The two main questions we want to address are: 1) what are the physicochemical characteristics of nanomaterials that drive their entry into cells? And, 2) can we design nanomaterials in order to achieve selective mode of entry into cells? The results will focus on carbonaceous nanoparticles, including a new class of compounds, carbonaceous quantum dots, which have recently emerged and ignited tremendous research interest. Their favorable characteristics include size- and wavelength-dependent luminescence, resistance to photobleaching, bio-conjugation, and functionalization to produce chiral nanostructures. Carbon-based quantum dots show promise in areas such optoelectronics, catalysis, bioanalysis and drug delivery. Atomistic simulations in conjunction with precise chemical and biophysical experiments are the distinguishing characteristics of this effort. Molecular dynamics simulations will examine the effects of nanoparticles parameters, such as size and chemical composition, on the entry mode of nanoparticles into cells. A conceptual framework is presented that envisions possible routes for the design of nanomaterials for nanomedicine applications.