Research Interests: Predrag S. Krstic

My multidisciplinary scientific background in theoretical studies of atomic and molecular physics, chemistry and physical chemistry, nanophysics, and biophysics is well suited for empowering a predictive theory, filling the gaps in understanding of the phenomena and explaining and integrating the experiments and theory in this application. I am applying multiscale theoretical methods, ranging from quantum mechanics (in fs and subnanometer-nanometer scale) and computational quantum chemistry, through the classical atomistic approach in molecular dynamics of nanofluids/nanomaterials , metalo-organic interfaces, DNA polymers and electrolytes (tens of ns, tens of nanometers), to continuum electrodynamics (Poisson-Planck-Nernst-Stokes) of liquid/solid media, ion transport, electro-osmosis, diffusion. The availability of the NCCS computational resources at ORNL NICS computational resources of University of Tennessee enables me with efficient tools in realization of the theoretical/computational research proposed in this application. I have a significant experience in leading of theoretical research at the several MHGRI research grants with ORNL, ASU and Yale U., and in collaborating with experimental scientists in the physical methods for the DNA sequencing.

My strong research interest has been in the processes at plasma - material interface, in the regime of interest for materials facing fusion plasma as well as plasma-mediated synthesis of nanoparticles. Particular focus has been the evolution of a collision cascade in the material upon slow impacts of ions, atoms and molecules of carbon, lithium, tungsten and mixed surfaces, changing morphology of the target material, and inducing various chemical reactions. Using modeling tools of quantum-classical and classical molecular dynamics, and bond-order potentials, we have studied chemical sputtering, reflection, sticking, penetration, retention, as well as nano-nucleation and growth of the nanostructures in function of the surface structure, of a state of a Monte-Carlo impact particle, of temperature and impact fluence, in a simulation cells of many thousands atoms.

My long-term interests and activities have been toward understanding of inelastic end elastic quantum dynamics in nearly adiabatic heavy particle collisions, involving ions, atoms and molecules. To describe multitude of various processes, from electronic transitions, to ro-vibrationally resolved collisions, involving processes of charge transfer, excitation, ionization, dissociation and association, considered at the “same footing” whenever possible, a number of methods were developed or adopted, from fully quantum-mechanical to semiclassical and classical approaches. Choice of the collision constituents and the parameters has been often determined by the needs in modeling of the fusion edge and astrophysical plasmas. By the same token the cross sections have been calculated in the comprehensive form, with the controlled accuracy whenever possible, scanning wide ranges of collision energies and underlined processes.

Multiphoton processes, mainly in nonperturbative strong filed regime, and mainly multiphoton ionization, have been my interest in theoretical atomic physics for a few decades. Motion of a bound or a free electron in the ultrastrong laser field is relativistic, which has for a consequence an effective change of the electron rest mass (nonrelativistically seen as a ponderomotive potential) as well as strong beyond-dipole effects. Particularly exciting in ionization in the limit of strong laser stabilization of atoms

against ionization in the limit of strong laser fields. Fully understand a role of electron-electron correlations in a few-electron dynamical system, particularly when interacting with photons. This underlines a need for development of a computationally highly intensive tools for numerical solution of the multielectron Schrodinger equation in dynamical regime, including methods of computational chemistry, various time-propagation and variable-step space discretization schemes, and quantum-classical molecular dynamics.