Computational Methodology For Resonant Nano-Plasma Theranostics For Cancer Treatment

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We describe a program of computational nanospectroscopy to employ the atomic, molecular, and plasma physics of atomic resonance formation and subsequent Auger fluorescence processes of electron ejection and photon emission for in vivo diagnostics and therapy of cancerous tumors. The methodology relies of large-scale atomic computations and modeling to predict the positions and strengths of resonance features in heavy high-Z elements such as Platinum and Gold delived to tumor sites as nanoparticles. These resonance features can be targeted via X-ray absorption, followed by many pathways for the breakup of the resultant Auger processes. The theoretical computations will help guide mono-energtic X-ray sources, such as the Electron-Beam-Ion-Traps, to target resonance complexes in specific energy ranges, and thereby induce in situ secondary
(a) electron ejecion via autoionization leading to DNA strand breakups, and
(b) X-ray emission, both predominatly localized at the tumor site.
The methodology entails: (I) Large-scale computations for resonance complexes in high-Z nanoparticle elements or molecular compounds using the powerful Relatvistic R-matrix and the COLUMBUS packages of codes from quantum chemistry, and (II) Modeling of nano-plasma opacities, attenuation coefficients, and numerical simulation of spectral features, to support an integrated system for Resonant Nano-Plasma Theranostics for potential cancer diagnostics and therapy

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