IIT Bombay INSPIRE fellow developing quantum chemistry based software useful for radiation therapy

Recipient of the INSPIRE Faculty Award instituted by Department of Science & Technology, Dr. Achintya Kumar Dutta from IIT Bombay along with his research group is working to develop new methods for quantum chemistry and implement them in efficient and free software to study electron attachment to aqueous DNA which has big implications in radiation therapy-based treatment of cancer.

Quantum chemistry is one of the new branches of chemistry which tries to understand the chemical properties of atoms and molecules without performing a lab experiment. Instead, in quantum chemistry, the Scientists try to solve the Schrödinger equation for the molecules, and it gives every measurable quantity about that particular molecule, without actually doing the measurement. However, the mathematical equations resulting from the application of the Schrodinger equation are very complicated and can only be solved using computers. Therefore, one needs to develop new theories and write efficient computer programs to solve these equations.

Indian scientists are at the forefront of the new theory development for quantum chemistry. However, the progress in translating those theories into practically useable computer software is somewhat limited. This is particularly surprising in the view of having a thriving Indian IT industry and extremely talented software professionals who are of global repute.

Dr. Dutta's research group in IIT Bombay is a collaboration of chemists, computer scientists, and engineers who are united towards a common goal of development of efficient quantum chemistry methods and free software, which can be routinely used by scientists all over the globe to solve their chemistry problems.

"My inspire fellowship has allowed me to establish a state of the art computing facility for developing and testing a new and efficient quantum chemistry software. It also allows me to train

quality manpower from all over India who can contribute to the further progress of Indian science." tells Dr Dutta

The efficiency of these newly developed quantum chemistry methods allows the research group to solve the Schrodinger equation for the attachment of electrons to DNA in the presence of the bulk aqueous environment. The deoxyribonucleic acid or DNA is the carrier of genetic information in human body, and electron attachment to DNA is one of the crucial steps in radiation damage to human cells. His team has shown that the electron attachment to DNA solvated in bulk water happens through a doorway mechanism, and the presence of the aqueous environment allows this electron attachment to take place at an ultrafast time scale. This newly proposed mechanism of electron attachment to aqueous DNA has big implications in radiation therapy-based treatment of cancer.

This study can help in the development of a new class of radio-sensitizers, which makes tumor cells more sensitive to radiation therapy and thereby protects the normal cells. Computational modeling can greatly reduce the development cost of new radio-sensitizers, both in terms of money and time.

Dr. Dutta wants to use the inspire fellowship to further develop new quantum chemistry methods, benchmark efficient computational protocols to study radiation damage to genetic material and pursue science for the betterment of our society and humankind.

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