1154-VN-2168   **Adnan Sljoka*** (`adnan.sljoka@riken.jp`). *Rigidity of graphs and applications to protein signalling and experimental design.*

To understand how proteins function one must examine their internal flexibility and dynamics. One critical way proteins regulate their function is through a phenomena known as 'allostery' which has been coined as 'second secret of life'. Allostery is a universal phenomena which involves regulation and/or signal transduction induced by a perturbation at one site on the protein which is a topographically distinct site from an active site. The molecular mechanisms that give rise to allostery are still poorly understood. In this talk, we treat a protein as a molecular multigraph where vertices represent atoms and edges various molecular bonding and non-bonding constraints. Molecular theorem in rigidity theory prescribes a combinatorial characterization of rigidity and flexibility which allows us to rapidly decompose a protein graph into rigid and flexible connection. Extending this theory, we have developed mechanistic models of allostery as transmissions of rigidity across molecular graphs. Recently, rigidity transmission allostery theory and algorithms have been used to decipher allostery in enzymes, membrane proteins and to guide biochemical NMR experiments in protein design (Sljoka, Science 2017, Nature Communication 2018, Journal of American Chemical Society 2019). (Received September 17, 2019)