



Padmesh Anjukandi
Ph.D., Massey University, New Zealand
Assistant Professor, Chemistry
padmesh@iitpkd.ac.in, 04923-226419
<https://iitpkd.ac.in/people/padmesh>



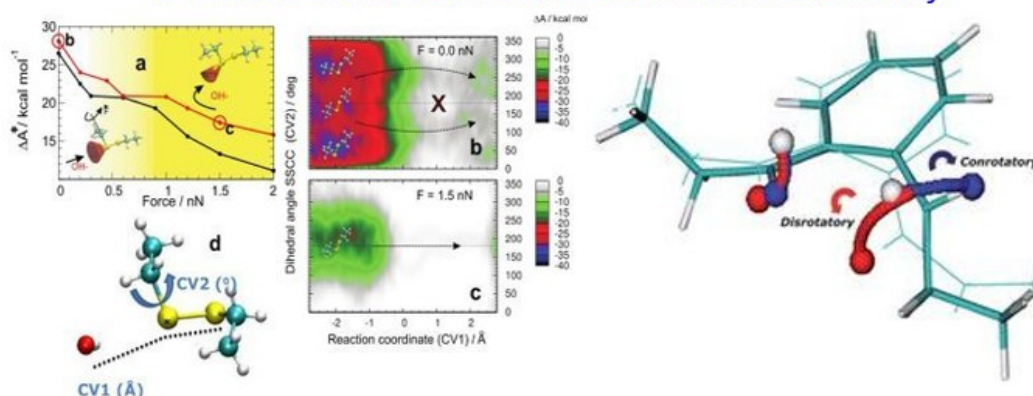
Research Interests

- Mechanochemistry of ring opening reactions.
- Bond breaking mechanisms of protein disulfides.
- Folding mechanisms in proteins.
- Organic electronic materials.

Brief Summary of Research

My research includes the theoretical study of folding mechanisms and disulfide bond making/breaking mechanisms as those in specific proteins. Calculating and simulating the mechanochemical reactions has been another area of interest. Main techniques that I use are *ab-initio* methods, Molecular dynamics approach, combined *ab-initio* molecular dynamics approach and advanced sampling techniques. I have currently two Ph. D. students at IITPKD and six masters students have submitted their thesis under my guidance as a part of their M.Sc. Program.

Disulfide bond reductions & Mechanochemistry



Projects

- Principle investigator for the project titled "On The Role of Proton Transfer in Triggering Disulfide Bond Reductions in Biological Systems – A Computational Approach (project reference no. YSS/2015/001956)" has been approved by Science and Engineering Research Board (SERB) for funding over a period of three years

Recent Publications (Full list of publications: <https://iitpkd.ac.in/people/padmesh>)

- P. Dopieralski, J. Ribas-Arino, **P. Anjukandi**, M. Krupicka and D. Marx; Unexpected mechanochemical complexity in the mechanistic scenarios of disulfide bond reduction in alkaline solution, *Nature Chemistry*, 9, 164-170, 2017.
- **P. Anjukandi***, P. Dopieralski, J. Ribas-Arino and D. Marx; The Effect of Tensile Strength on the Conformational Free Energy Landscape of Disulfide Bonds, *PloS One*, 9(10): e108812, 2014.
- P. Dopieralski, J. Ribas-Arino, **P. Anjukandi**, M. Krupicka, J. Kiss, and D. Marx; The Janus-faced role of external forces in mechanochemical disulfide bond cleavage, *Nature Chemistry*, 5, 685-691, 2013.