



# OPEN TALK

21 July 2014

3:00 p.m.

Fermion

Speaker:

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Title:

**Role of residues in the stability of EF-hand loop I in Ca bound Calmodulin**

Abstract:

Ca modulated protein such as Calmodulin has a regulatory function in living cells. In other words, one can say that in order to regulate the influx of Ca in cells, the protein must bind with Ca. However the binding of Ca within a protein loop of Calmodulin is not well-investigated. We have studied within density functional theory, the calcium ion coordination in an EF-hand protein loop I of Calmodulin (Ca bound protein molecule) in vacuum. We have elucidated the roles played by both the coordinating and non coordinating residues in stabilizing the bipyramidal coordination geometry of the loop. We further shed light on the roles played by the coordinating residues, which are in accord with the various mutational studies on this protein. The role of non-coordinating residues will also be discussed. This study of metal ion coordination in a metalloprotein provides insight on how a metal ion stabilises within a protein core. Such an

understanding can be applied in the design of metalloproteins with preprogrammed properties.

We have now performed first-principles calculations on all the four loops of Calmodulin, taking into consideration implicit solvent. Very preliminary results will be mentioned. Also the dynamics of the coordination process in the protein loops of Calmodulin is now being explored using Molecular dynamics code such as SIESTA/VASP .

#### REFERENCES:

[1] S. Sikdar, M. Ghosh, M. De Raychaudhury and J. Chakrabarti, Chemical Physics Letters, Vol. 605-606, pp. 103-107 (2014)

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