

Title: On the Optical Properties of L-glutamine and Pyroglutamic acid

Abstract: In recent experiments[1], amyloid fibrils and similar protein crystal structures has been found to absorb light near the ultra violet range and emit in the visible even in the absence of the aromatic residues and pi-conjugated bonds. The molecular origin of this peculiar florescence is need to be understood. Previous theoretical studies[1, 2] on model amyloid systems shows that the proton transfer happens along specific hydrogen bonds, coupled to the optical absorption of these systems.

In this work we present our studies on the behavior of hydrogen bonded rich systems, mainly L-glutamine and pyroglutamic acid structures. We showed that the structures with strong hydrogen bond undergoes with frequent proton transfer, absorbs at lower energies. Our calculations reflects that in these hydrogen bond rich systems, the proton transfer events are coupled to the vibrational modes of the nearby heavy atoms. A significant electron delocalization is associated with proton shuffling along the hydrogen bond suggesting the hypothesis that the peculiar photo physics of these system is related to the frequency of the proton motion.

References

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- [2] L Grisanti, D Pinotsi, R Gebauer, GSK Schierle, AA Hassanali *Physical Chemistry Chemical Physics* 19 (5), 4030-4040