MAR13-2012-000935

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Challenges for understanding protein aggregation through computer simulations[1]

NORMAND MOUSSEAU, Université de Montréal

The first computer simulations of protein aggregation were performed a little more than decade ago. Over the years, the community of computer biochemists, chemists and physicists has grown considerably and the simulations becoming more realistic and often closer to experiments, due both to a better understanding of the onset of aggregation and to ever more powerful computers. In view of this expansion both in terms of papers and system size, what have been the real contribution of these simulations to our understanding of amyloid diseases? In this talk, I will present a personal view of the progress that has been accomplished over the last decade. I will aslo discuss some of the challenges that must still be overcome for computer simulations to move to the next level of contributions to this fundamental problem.

[1]This work is supported by NSERC and the Canada Research Foundation.