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Coarse-Grained computer simulations of Alzheimer's beta-amyloid peptides, using the Mercedes-Benz Hydrogen Bond Potential

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Protein aggregation is a medically relevant phenomenon that can lead to protein-folding diseases such as Alzheimer's and Prion's. The aggregation process is largely determined by hydrogen bonds (HB), involving hundreds of peptides, over a period of days or even months. This rules out molecular dynamics (MD) simulations of all-atom protein models in explicit solvents. However, coarse-grained models of protein aggregation must accurately represent HB. This work considers the coarse-grained model used by Head- Gordon and coworkers to study the beta-amyloid (Aβ) peptides that forms plaques in
Alzheimer's diseases [1]. The model represents one amino-acid residue by a single bead, and used the Mercedes-Benz (MB) model to describes backbone HB. This has been adapted to study residue 25 to 35 of the peptide, Aβ_{25-35}, which is believed to be the most
toxic stretch of Aβ. Preliminary work has obtained data on Langevin dynamics of 100 Aβ_{25-35} in a 100A ×100A ×100A box. The model peptides will be immersed in the MB
water model of Dias and coworkers [2], used previously to study cold denaturation of proteins. The final model will be used to accurately identify the structure of Aβ
intermediates believed to the neurotoxin agents in Alzheimer's disease.
[1] Hui, Fawzi, Head-Gordon, Proteins 70, 626 (2008)
[2] Dias, Alla-Nissila, Grant, Kartunnen, J. Chem. Phys. 131, 054505 (2009)

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