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$\alpha-$synuclein under the magnifying glass. Insights from atomistic and coarse-grain simulations. IOANA M. ILIE, University of Twente, DIVYA NAYAR, Technical University Darmstadt, WOUTER K. DEN OTTER, University of Twente, NICO F. A. VAN DER VEGT, Technical University Darmstadt, WIM J. BRIELS, University of Twente, UNIVERSITY OF TWENTE COLLABORATION, UNIVERSITY OF DARMSTADT COLLABORATION — Neurodegenerative diseases are linked to the accumulation of misfolded intrinsically disordered proteins in the brain. Here, we use both all-atom and coarse-grain simulations to explore the intricate dynamics and the aggregation of α-synuclein, the protein implicated in Parkinson's disease. We explore the free energy landscapes of α-synuclein by using Molecular Dynamics simulations and extract information on the structure of the protein as well as on its binding affinities[1]. Next, to study the aggregation, we proceed with representing α-synuclein as a chain of deformable particles that can adapt their geometry, binding affinities and can rearrange into different disordered and ordered structures[2,3]. We use Brownian Dynamics to simulate the translational and rotational motions of the particles[4], as well as their interaction properties[2]. The simulations show valuable insight into the internal dynamics of α-synuclein[1] and the formation of ordered and disordered aggregates[2]. In addition, the study is extended to investigate the attachment and folding of a protein to a fiber[3]. [1]I.M.Ilie, D.Nayar, W.K.den Otter, N.F.A.van der Vegt & W.J.Briels, in prep [2]I.M.Ilie, W.K.den Otter and W.J.Briels, JCP 144, 085103 (2016) [3]I.M.Ilie, W.K.den Otter and W.J.Briels, in prep [4]I.M.Ilie, W.J.Briels and W.K.den Otter, JCP 142, 114103 (2015)

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