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# Transition metal ions interactions with intrinsically disordered proteins

**Orkid Coskuner**
University of Texas, USA

Metals are intrinsic in nature and are necessary for vital biological functions. Metals are required for life and health in small amounts but are toxic if intake occurs in excessive amounts. Zinc, iron, and copper functions as co-factors or as toxic ions. These metals bind to intrinsically disordered fibrillogenic proteins that are at the center of neurodegenerative diseases. Amyloid-β is at the center of Alzheimer's disease; it is known that the amyloid-β(1-40) fragment is the dominant and the amyloid-β(1-42) is the most toxic fragment. Moreover, α-synuclein is at the center of Parkinson's disease. Metal ions, such as copper and zinc bind to these intrinsically disordered fibrillogenic proteins and affect their aggregation processes. Fast conformational changes, solvent effects and rapid aggregation processes provide challenges in the direct measurements using conventional experimental tools. Theoretical tools, i.e., molecular dynamics simulations along with state-of-the-art thermodynamic calculations can provide atomic level insights with dynamics into the structures of these metalloproteins. However, potential functions necessary for these investigations are currently lacking. We use all three levels of physics; quantum and statistical mechanics and thermodynamics for developing the lacking theoretical tools and we apply these in the theoretical studies of intrinsically disordered fibrillogenic metalloproteins for understanding their structures and free energy landscapes at the atomic level with dynamics. These studies are crucial for providing a basic understanding to the structure and function relationship of metalloproteins at the center of neurodegnerenative diseases and can be used in finding and designing more efficient treatments and metal ion chelators.

## Biography

Orkid Coskuner has completed her Ph.D. studies at the Universitaet Zu Koeln in Germany within three years. She has worked as a postdoctoral scientist at the Johns Hopkins and Stanford Universities and National Institute of Standards and Technology. She is an assistant professor of Chemistry and Neurosciences since 2009 at The University of Texas at San Antonio. She has developed and published many various new theoretical methods and their applications in deputed Journals and book chapters; she is also editorial board member of repute. She is the PI of the BioProtMet group at The University of Texas at San Antonio.

Orkid.CoskunerWeber@utsa.edu