

# **Zn induced structural aggregation patterns of $\beta$ -amyloid peptides by first-principle simulations and XAS measurements**

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We show in this work that in the presence of Zn ions a peculiar structural aggregation pattern of  $\beta$ -amyloid peptides in which metal ions are sequentially coordinated to either three or four histidines of nearby peptides is favored. To stabilize this configuration a deprotonated imidazole ring from one of the histidines forms a bridge connecting two adjacent Zn ions. Though present in zeolite imidazolate frameworks, remarkably in biological compounds this peculiar Zn–imidazolate–Zn topology is only found in enzymes belonging to the Cu,Zn-superoxide dismutase family in the form of an imidazolate bridging Cu and Zn. The results we present are obtained by combining X-ray absorption spectroscopy experimental data with detailed first-principle molecular dynamics simulations.

**Presenter:** MINICOZZI, Velia