

Abstract Submitted
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Comparing potential copper chelation mechanisms in Parkinson's disease protein FRISCO ROSE, MIROSLAV HODAK, JERRY BERNHOLC, CHiPS/NCSU — We have implemented the nudged elastic band (NEB) as a guided dynamics framework for our real-space multigrid method of DFT-based quantum simulations. This highly parallel approach resolves a minimum energy pathway (MEP) on the energy hypersurface by relaxing intermediates in a chain-of-states. As an initial application we present an investigation of chelating agents acting on copper ion bound to α -synuclein, whose misfolding is implicated in Parkinson's disease (PD). Copper ions are known to act as highly effective misfolding agents in α -synuclein and are thus an important target in understanding PD. Furthermore, chelation therapy has shown promise in the treatment of Alzheimer's and other neuro-degenerative diseases with similar metal-correlated pathologies. At present, our candidate chelating agents include nicotine, curcumin and clioquinol. We examine their MEP activation barriers in the context of a PD onset mechanism to assess the viability of various chelators for PD remediation.

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