
Abstract

Metal ions are a tempting tool for organisms thanks to the diversity of functions they have to offer, if they can be distinguished properly. Examining metal-ion selectivity computationally is challenging mainly due to complexity of electronic structure and solvation effects. A DFT-based protocol for predicting metal-ion selectivity of metal-binding systems was developed. The most essential part of the thesis is discussion of the magnitudes and sources of inherent errors, both for metal-ion complexes and small peptides. The thesis connects the work of four original papers. It includes computational and experimental benchmarks, a case-study validating the computational protocol for obtaining energetic and structural insights, and attempts applying the protocol to peptidic systems.