

Mechanistic study of Pb(II) removal by activated carbon: Spectroscopy, DFT calculations, and the effect of co-existing ions

QIANTAO SHI¹, VALENTINA PRIGIOBBE¹, AND
XIAO GUANG MENG^{1*}

¹ [¹Center for Environmental Systems, Stevens Institute of Technology, Hoboken, New Jersey 07030, United States¹
*correspondence: xmeng@stevens.edu]

Lead is a highly toxic element that occurs in drinking water as a divalent ion (Pb(II)) due to leaching from service pipes in the potable water network. Point-of-use (POU) filters have been widely applied to remove Pb(II) from tap water. The major media used in POU filters consist of activated carbon (AC); however, the mechanism of Pb(II) removal by AC is yet to be fully elucidated. In this study, the interactions of Pb(II) with functional groups on AC were investigated using spectroscopic measurements and first principle calculations. Fourier transform infrared (FTIR) spectroscopy analyses indicated that Pb(II) formed complexes with phenol and carboxyl groups on the AC surface. Coordination analysis for Pb(II) on AC by extended X-ray absorption fine structure (EXAFS) suggested the existence of monodentate and bidentate mononuclear configurations, with an average interatomic Pb(II)-C distance of 3.12 Å. Possible bidentate mononuclear Pb(II) carboxyl and monodentate mononuclear Pb(II) phenol complexes on AC were confirmed by density functional theory (DFT) calculations. Competitive adsorption behavior was observed between Pb(II) and calcium (Ca(II)) due to their similar complexation behavior. By contrast, co-existing sulfate (SO₄²⁻) and dihydrogen phosphate (H₂PO₄⁻) formed ternary complexes with Pb(II) on the AC surface, enhancing its adsorption. Based on these observations, a new surface complexation model of Pb(II) adsorption onto AC was formulated. This study reveals the molecular-level mechanism of Pb(II) removal by AC, which is helpful for gaining a fundamental understanding of the process and prediction of Pb(II) removal by POU filters.