

Abstract Submitted  
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**Actinides in Solution: Disproportionation, Strong Correlations, and Emergence**<sup>1</sup> BRAD MARSTON, STEVEN HOROWITZ, Brown University — Plutonium in acid solutions can be found in oxidation states III through VI. There is a striking near perfect degeneracy of the reduction-oxidation (redox) potentials, each being about 1 volt. Neptunium is the only other element that approaches this degree of degeneracy. One consequence of the redox degeneracy is a marked tendency of plutonium ions to disproportionate; up to four different oxidation states can coexist simultaneously in the same solution, greatly complicating the environmental chemistry of the element. While the degeneracy could simply be a coincidence, it could also be the manifestation of a higher-level organizing principle at work. Other systems that exhibit disproportionation raise the possibility of an emergent negative-U attractive interaction. The hypothesis is tested by combining first-principles relativistic density-functional calculations using the Amsterdam Density Functional (ADF) package with exact diagonalizations of Hubbard-like models of the strong correlations between the actinide 5f electrons.

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