

Distinguished Seminar Series in Materials Theory

“Electronic structure of nuclear materials from first principles”

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Friday, April 23, 2010
11:00 a.m.
4500N/Weinberg Auditorium

Abstract:

Actinide oxides have always played a dominant role in the nuclear fuel cycle, and with respect to the development of generation IV fast breeder reactors, actinide carbides and nitrides, are being investigated as candidate future fuel materials. Studying the electronic properties of nuclear materials provides important insight into a variety of highly debated issues such as fuel performance, environmental impact, and waste disposal. We use the self-interaction corrected local spin density (SIC-LSD) approximation to determine the groundstate electronic structure of these compounds from first principles. Our study reveals that apart from having a major impact on the nature of the anion-actinide bond, the degree of 5f-electron localization is a determining factor in the stability of actinide oxides towards oxidation. The predicted considerable changes in electronic structure from the early to the late actinides will be discussed with respect to the resulting differences in the thermophysical and chemical properties of the corresponding nuclear materials.

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