Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Electrophobic interaction induced impurity clustering in metals GUANG-HONG LU, HONG-BO ZHOU, School of Physics, Beihang University, J AGUIAR, National Renewable Energy Laboratory, FENG LIU, Department of Materials Science and Engineering, University of Utah — Helium is a typical impurity in metals, which is produced from transmutation reactions in both fission and fusion. It is well known that He atoms are energetically favorable clustering with each other, resulting in mechanical property degradation of metals, which is originated from the self-trapping of He. Here, we introduce the concept of electrophobic interaction, analogous to hydrophobic interaction, for describing the behavior of impurity atoms in a metal, a solvent of electrons. We demonstrate that there exists a form of electrophobic interaction between impurities with closed electron shell structure, which governs their dissolution behavior in a metal. Using He, Be and Ar as examples, we predict by first-principles calculations that a clustering energy due to the electrophobic interaction follows a universal power-law scaling with the number of atoms (N) dissolved in a free electron gas, as well as W or Al lattice, as Ec $\propto$ (N$\hat{}$2/3 – N). This new concept significantly advances our fundamental understanding and capacity to predict the solute behavior of impurities in metals, a useful contribution to be considered in future material design of metals for nuclear, metallurgical, and energy applications.

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Date submitted: 29 Oct 2016 Electronic form version 1.4