Abstract Submitted
for the NWS05 Meeting of
The American Physical Society

Beyond the Arbitrariness of Ionic or Covalent Radii: Determination of Effective Atomic Radii in Solids from Electron Density RAFAL BACHORZ, IVAN YAKOVKIN, JOHN JAFFE, MACIEJ GUTOWSKI, Pacific Northwest National Laboratory — Effective atomic radii, net atomic charges, and projected densities of states are useful parameters for the evaluation of properties of solids. Within typical plane-wave expansion methods, atomic radii are required to carry on the population analysis. Unfortunately, there is no unique recipe how to determine effective radii. Tabulated sets of radii are commonly used, which do not reflect the specifics of chemical bonding in a particular solid. When using tabulated radii one frequently recognizes that a significant fraction of electron density is not assigned to any atom and the sum of projected densities of states (PDOS) poorly reproduces the total density of states (DOS). We propose a variational approach based on the charge density in the unit cell to determine effective atomic radii. The radii are constrained by a condition that the sum of volumes of spheres assigned to atoms should be equal to the volume of the unit cell. The radii are considered to be optimal when the total electron charge contained in a volume that is spanned by the atomic spheres has the maximal value. The optimal radii are system dependent and illustrate the effect of environment on charge distribution on each atom.

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Date submitted: 11 Apr 2005 Electronic form version 1.4