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Novel approach to electron partitioning and definitive oxidation state assignment in solids LAI JIANG, SERGEY LEVCHENKO[1], ANDREW RAPPE, University of Pennsylvania — Oxidation state of a atom is usually defined by partitioning electrons to the nucleus based on charge density distribution, which inherits uncertainty from the probabilistic nature of wavefunctions. Here we propose a first principle approach to electron partitioning in insulating solids based on wavefunction topology. By calculating polarization change upon shifting an atomic sublattice to its periodic image, the charge transferred during nuclei displacement can be derived. To rationalize, in Wannier representation the Berry's phase polarization is directly related to the position of Wannier Center (WC) of each band, therefore a quantized charge flow is determined by the number of WCs that move together with (*i. e.* belong to) the nucleus. We provide both rigorous mathematical definition of oxidation states in this scheme and results from calculations of various sample systems that corroborate with oxidation states assigned by conventional chemical insight.

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