Geometric Phases, Distribution of Electron Charge Centers, Wannier Functions and Bonding in Materials

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We describe a scheme to determine non-abelian geometric phases [1] of Bloch electrons in the frame-work of density functional theory and discuss their use and implications to the theory of polarization and construction of Wannier Functions [1, 2]. Through projection of Wannier functions onto atomic orbitals, we introduce concepts of Bond Orbital Overlap Population and Bond Overlap Position Population. Using these constructs, we show that the origin of anomalously large Born dynamical charges in d^0 transition metal oxides, such as ferroelectrics, is in the long-range transfer of small electronic charge between transition metal ions through the bridging oxygen ion, analogus to double exchange mechanism in ferromagnets [3]. Finally, we present a new gauge invariant functions, Distribution of Electron Charge Centers (DECC) that provides partitioning of extended charge density in crystals, yielding a description of electronic structure in terms of average position of electrons [4]. This provides a natural picture of bonding, with a general and precise definition of an $n-$electron $m-$centre bond.

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