A Self-Consistent Atomic Deformation Model for Bonding Charge

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An approach to first-principles studies of electronic structure and total energy based on localized densities, called self-consistent atomic deformation (SCAD), is presented. In this method the densities are obtained by solving one-electron Schrödinger's equations, one for each atomic site, whose potentials are determined variationally from the total energy. A local-density approximation is used to account for exchange and correlation energy. Kinetic energy contributions due to overlapping densities are included using the Thomas-Fermi approximation. This approach has been applied to calculate various properties of crystals with bonding having ionic character. In the SCAD method bonding charge can have a different origin from that derived in a band structure calculation. In particular, bonding charge, resulting from a linear combination of atomic orbitals in a band structure approach, results, in the SCAD method, from non-spherical deformation of the negative ions. We illustrate this with results from a simple example, silicon carbide. Results for Al_2O_3 will also be presented.