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Self Consistent Calculations of Electronic Properties of Systems with an Energy or a Band Gap DIOLA BAGAYOKO, LASHOUNDA FRANKLIN, Department of Physics Southern University and A&M College, Baton Rouge, LA 70813, CHINEDU EKUMA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, YURIY MALOZOVSKY, Department of Physics Southern University and A&M College, Baton Rouge, LA 70813
— We re-examine the process of performing self consistent calculations of electronic and related properties of finite systems (with an energy gap) and of crystals with a band gap. This work applies to calculations utilizing density functional and X? potentials and to other approaches that entail solving a system of inherently coupled equations. In particular, the local density approximation (LDA) is defined by a system of equations that reduces to two equations upon the selection of Vxc. We show how the Bagayoko, Zhao, and Williams (BZW) method solves the relevant system of equations and leads to results in excellent agreement with experimental ones. We discuss such results for w-ZnO, rutile TiO2, w-CdS, zb-CdS, zb-InP, Ge, Ca B6, and other materials. Work funded by the National Science Foundation, through LASiGMA [NSF AwardEPS-1003897 and No. NSF (2010-15)-RII-SUBR], LONI [Award No. 2-10915], and Ebonyi State, Federal Republic of Nigeria.

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