Special Guest Lectures

A Mathematical Solution to the Theoretical Underestimation of Energy and Band Gaps and Applications to the Search of Novel Materials

Diola Bagayoko, Southern University

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Abstract:
Most density functional theory (DFT) calculations find band gaps that are 30-50 percent smaller than the experimental ones. Some explanations of this serious underestimation by theory include self-interaction and the derivative discontinuity of the exchange correlation energy. Several approaches have been developed in the search for a solution to this problem. Most of them entail some modification of DFT potentials. The Green function and screened Coulomb approximation (GWA) is a non-DFT formalism that has led to some improvements. Despite these efforts, the underestimation problem has mostly persisted in the literature. Using the Rayleigh theorem, we describe a basis set and variational effect inherently associated with calculations that employ a linear combination of atomic orbitals (LCAO) in a variational approach of the Rayleigh-Ritz type. This description concomitantly shows a source of large underestimation errors in calculated band gaps, i.e., an often dramatic lowering of some unoccupied energies on account of the Rayleigh theorem as opposed to a physical interaction. We present the Bagayoko, Zhao, and Williams (BZW) method [Phys. Rev. B 60, 1563 (1999); PRB 74, 245214 (2006); and J. Appl. Phys. 103, 096101 (2008)] that systematically avoids this effect and leads (a) to DFT and LDA calculated band gaps of semiconductors in agreement with experiment and (b) theoretical predictions of band gaps that are confirmed by experiment. Unlike most calculations, BZW computations solve, self-consistently, a system of two coupled equations. DFT-BZW calculated effective masses and optical properties (dielectric functions) also agree with measurements. We illustrate ten years of success of the BZW method with its results for GaN, C, Si, 3C-SIC, 4H-SiC, ZnO, AlAs, Ge, ZnSe, w-InN, c-InN, InAs, CdS, AlN and nanostructures. We conclude with potential applications of the BZW method in molecular and semiconductor engineering to inform and to guide the design and fabrication of semiconductor and nanostructure-based devices. Note: 338 Johnston is Axis Grid viewing. Live presentation is at 218 J.B. Moore Hall at Southern University.

Speaker's Bio:
Dr. Diola Bagayoko is Southern University System Distinguished Professor of Physics, Adjunct Professor of Science and Mathematics Education, and Director of the Timbuktu Academy. He earned the BS degree in Physics and Chemistry from the Ecole Normale Supérieure (ENSup) of Bamako, Mali, the MS in the Physics from Lehigh University, Bethlehem, Pennsylvania, and the Ph.D. in condensed matter theory from Louisiana State University under the supervision of the late Boyd Professor Joseph Callaway. Dr. Bagayoko has had four years of formal training in the arts and science of teaching and learning at the ENSup (1969-73). More details are available on the web (http://www.phys.subr.edu/faculty/bagayoko) on the teaching, mentoring, research, program development, and service activities and results of Bagayoko. His teaching and mentoring work and results are partly attested to by the internationally recognized success of the Timbuktu Academy he has directed from 1990 to present (http://www.phys.subr.edu/timbuktu.htm). This Academy won the 2002 US Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring. This claim to success is also borne out in part by two distinct commendations by national experts consulted by the Louisiana Board of Regents in 1995-96 and in 2000-01 and particularly by the closing of the achievement gaps between hundreds of pre-college and college African American Scholars of the Academy and any other ethnic groups! His K-16 involvement and accomplishment portfolio cannot be fully described in a few lines. In addition to the work at the Timbuktu Academy, it includes leadership in elementary to college education reform, teaching high school Physics at the Southern University Laboratory School, implementing the educational outreach component of LaSPACE (1992-2000), extensive speaking to K-12 students and teachers for the SOS program of Louisiana EPSCoR, serving as the director of campus coordination for LS-LAMP (1996-2005, www.ls-lamp.org; LS-LAMP was directed by Dr. Robert L. Ford from 1996 to 2003), and directing a major STEM pipeline program (www.phys.subr.edu/pipelines/_ whose core activity is the implementation of GLOBE (www.globe.gov) in more than 20 Louisiana schools. Of his more than one hundred twenty (120) publications in a mostly undergraduate department, over seventy (70) are in physics (condensed matter theory) and over forty (40) are on teaching, mentoring, and learning. Bagayoko successfully managed over $1,000,000 of educational, research, and infrastructure development funding per year from 1993 to 1998. From 1998 to 2005, he is averaging well over $2,000,000 per year. He is an active member of several national and international professional organizations, including the American Physics Society (APS), the National Society of Black Physicists (NSBP), New York and Louisiana Academies of Science. He has served on several state and national committees, including the Louisiana EPSCoR and LEQSF Planning committees and the Science Advisory Committee of the National Association for Equal Opportunity (NAFEO) in Higher Education. Bagayoko has served as consultant for the Southern Regional Education Board (SREB), the National Association for Equal Opportunity (NAFEO) in Higher Education, the United Nations Educational, Scientific, and Cultural Organization (UNESCO), the Louisiana Department of Education, and many universities and other organizations. His awards include Teacher of the Year, Chancellor's Research Excellence, Southern University System President's Faculty Excellence, and the Renaissance awards at SUBR; the Louisiana Governor's Award for Excellence in Educational Reform (1993); and the individual US Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring in 1996. The aim is to make some positive contributions and to set adequately high standards (judgment, character, effort, and results) for his students and children to surpass. Bagayoko routinely speaks of many individuals who gave him the opportunity. They include his parents, several pre-college and college teachers and mentors, some peers including Dr. Robert L. Ford, funding agencies, and others. "Luck is what happens when preparation meets, recognizes and acts on opportunity."

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