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凝聚态物理-北京大学论坛

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A Mathematical Solution to the Theoretical Band Gap Underestimation: *Predictive Calculations of Properties of Semiconductors and nanostructures*

Prof. Bagayoko

时间：3月25日（星期四）15:00－16:40

地点：北京大学物理大楼中212教室

Prof. Bagayoko, **Over 90 of the 150 relevant publications mostly deal with materials physics: electronic, cohesive, magnetic, optical, and other properties of metals, semiconductors, oxides, clusters, and nanotubes.**
Southern University System Distinguished Professor and Chairman, SUBR, January 2009 - present
Professor of Physics and Chancellor's Fellow, SUBR, 1994 – present
The Academy received the 2002 US Presidential Award for Excellence in SME Mentoring- (White House Ceremony on 03/18/03).
One of first 10 recipients of US Presidential Award for Excellence in Science, Mathematics, and Engineering (SME) Mentoring (September 25, 1996; Washington, D.C.)

Abstract: Most density functional calculations find band gaps that are 30-50% smaller than the experimental ones. We illustrate this fact with the examples of DFT calculated band gaps for ZnO, AlAs, Si, Ge, and wurtzite and cubic InN. We subsequently recall some popular explanations of the DFT band gap problems, i.e., self-interaction effects and derivative discontinuities of the exchange correlation energy. 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 the Hamiltonian .

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