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Physics Department Seminar

Friday March 2nd, 2001

11:00am in PhSc 105

"Implementation Of A Coulomb Hole Treatment Of Electron Correlations"

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Abstract:

Many formalisms dealing with correcting the fundamental gap in semiconductors exist in the literature, but their implementations often turn out to be computationally intensive. Based upon a general belief that the local density approximation (LDA) within density functional theory is the reason why the band gap is underestimated, one possible improvement would be to consider a better treatment of electron correlations. One proposed form is the Coulomb hole model which, according to recent quantum Monte Carlo results, plays a dominant role in electron correlations. We implemented one such Coulomb hole formalism and used it to replace the LDA correlation in our code. Our modifications resulted in the same level of computational effort as the LDA. Within this model, we will present results of testing done on several different elemental and compound crystals, with semiconducting or insulating properties.