Abstract Submitted
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Excited state calculations in solids by auxiliary-field quantum Monte Carlo[1] FENGJIE MA, SHIWEI ZHANG, HENRY KRAKAUER, College of William and Mary — We present an approach for ab initio many-body calculations of excited states in solids. Using auxiliary-field quantum Monte Carlo [2], we introduce an orthogonalization constraint with virtual orbitals to prevent collapse of the stochastic Slater determinants in the imaginary-time propagation. Trial wave functions from density-functional calculations are used for the constraints, and detailed band structures can be calculated. Results for standard semiconductors are in good agreement with GW calculations and with experiment. For the challenging ZnO, we obtain a fundamental band gap of 3.30(16) eV, consistent within the range of experimental measurements [3]. Applications to other systems are currently underway.

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[2]S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003)
[3]V. Srikant and D. R. Clarke, J. Appl. Phys. 83, 5447 (1998); S. Tsoi, X. Lu, A. K. Ramdas, H. Alawadhi, M. Grimsditch, M. Cardona, and R. Lauck, Phys. Rev. B 74, 165203 (2006); H. Alawadhi, S. Tsoi, X. Lu, A. K. Ramdas, M. Grimsditch, M. Cardona, and R. Lauck, Phys. Rev. B **75**, 205207 (2007)

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