For some time, density functional theory[1] was the main tool used in computational condensed matter physics due to its simplicity and relative computationally-inexpensive implementations, as well as its remarkable success in determining the elctronic properties of real materials. However, with the increase in availability of high-performance computational resources and the high interest in materials that exhibit properties beyond the scope of DFT, it is desirable to find and use methods that, while computationally expensive, offer greater accuracy. One area in which DFT has notoriously fallen short is the calculation of band gaps in many semiconductors and insulators. We have applied the hybrid-functional method in VASP[2] in which the exchange funcional is calculated partially from DFT and partially from the Hartree-Fock term, to the spinel $NiFe_2O_4$, a ferrimagnetic insulator, and to VO_2, a well-studied material with a metal-insulator transition accompanied by a structural rutile-monoclinic transition. In both systems, ordinary DFT cannot reproduce the observed properties, but we find good agreement with experiment using the HF method.

References

1. W. Kohn and L. J. Sham , Phys. Rev 140, A1133 (1965).
2. G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993); G. Kresse and J. Hafner, Phys. Rev. B 49, 14 251 (1994); G. Kresse and J. Furthmüller, Comput. Mat. Sci. 6, 15 (1996); G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996).