h) Highlights

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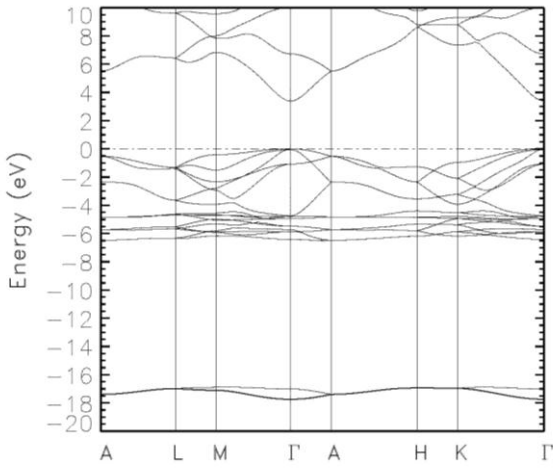
A Mathematical Pathway to Predictive Calculations of Properties of Materials

We solved self-consistently the *system of equations* defining the local density approximation. We obtained electronic energies and related properties of semiconductors in excellent agreement with experiment. *The situation is analogous to sounds and expected sound respectively from an unturned and a tuned guitar string.*

The benefits of the above approach to the semiconductor and nanotechnology industries cannot be overstated. The trials and errors that currently undergird the design and fabrication of devices can be mostly replaced by accurate theoretical predictions that can inform and guide the referenced design and fabrication.

Several individuals in our group at Southern University and A&M College in Baton Rouge (SUBR) contributed to various aspects of this work. They include D. Bagayoko and G. L. Zhao, the group leaders, L. Franklin, and C. E. Ekuma. The latest improvement of the computational method, made possible through LASiGMA funding [EPS-1003897 and NSF (2010-15)-RII-SUBR] dramatically enhanced the agreement between our calculated results and experimental ones. The robustness and totally ab-initio nature of the method immensely add to its intellectual merit in the resolution of long-standing disagreement between calculated energy and band gaps and experimentally measured ones. As noted in the preceding paragraph, this method permits theory to inform and to guide the design and fabrications of novel materials and nanostructure and semiconductor based devices.



Calculated electonic energy bands of zinc oxide (ZnO). The direct band gap at the gamma point is 3.4 eV.
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