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Gap engineering using Hellmann-Feynmann forces: method and applications[1] KIRAN PRASAI, Ohio University, PARTHAPRATIM BIAWAS, The University of Southern Mississippi, D. A. DRABOLD, Ohio University — Materials with optimized band gap are needed in many specialized applications. In this talk, we demonstrate that Hellmann-Feynman forces associated with the gap states can be used to find atomic coordinates that yield desired electronic density of states. Using tight-binding models, we show that this approach may be used to arrive at electronically designed models of amorphous silicon and carbon. We provide a simple recipe to include *a priori* electronic information in the formation of computer models of materials, and prove that this information may have profound structural consequences. We'll briefly discuss implementation of the method in ab-initio molecular dynamics simulations and highlight the latest feats of the method ranging from modeling amorphous semi-conducting materials to understanding the structure and properties of memory materials.

[1]K. Prasai, P. Biswas, and D. A. Drabold, Scientific reports, 5 (2015)

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